Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 03:28 PM EDT

PDB ID	:	8CTA
Title	:	Minimal 2:2 Ternary Complex between BI-224436 bound HIV-1 Integrase Catalytic Core Domain Dimer and Carboxy Terminal Domains
Authors	:	Gupta, K.; Van Duyne, G.D.; Eilers, G.; Bushman, F.D.
Deposited on	:	2022-05-13
Resolution	:	2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

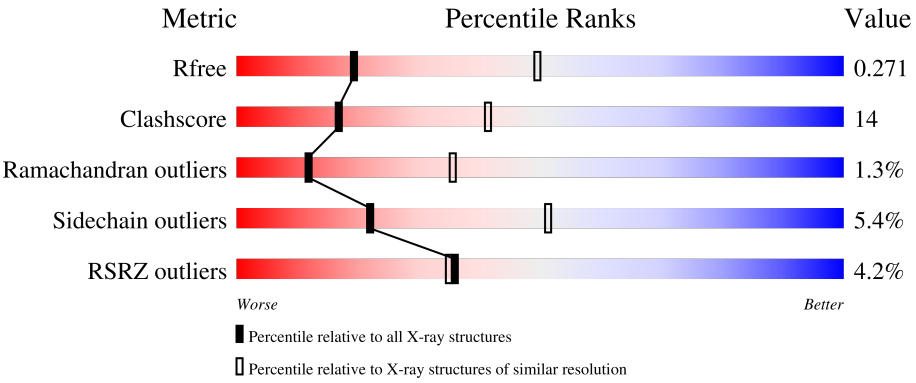
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	161	3% 61% 20% • 16%
1	B	161	2% 66% 17% • 14%
1	E	161	4% 63% 21% • • 12%
1	F	161	2% 66% 18% • 14%
1	I	161	2% 73% 14% • • 10%

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Mol	Chain	Length	Quality of chain
1	J	161	3% 61% 19% 16%
1	M	161	5% 76% 16% 6%
1	N	161	2% 62% 20% 15%
2	C	53	9% 36% 38% 11% 13%
2	D	53	4% 74% 15% 6% 6%
2	G	53	6% 57% 28% 8% 8%
2	H	53	9% 72% 17% 6% 6%
2	K	53	8% 55% 30% 13%
2	L	53	79% 15%
2	O	53	2% 58% 28% 9%
2	P	53	8% 66% 25% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	E	302	-	-	-	X
4	EDO	F	501	-	-	X	-
4	EDO	K	502	-	-	-	X
4	EDO	P	301	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12460 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1056	676	184	192	4			
1	B	138	Total	C	N	O	S	0	0	0
			1081	690	186	200	5			
1	E	141	Total	C	N	O	S	0	0	0
			1091	698	189	200	4			
1	F	138	Total	C	N	O	S	0	0	0
			1084	693	187	200	4			
1	I	145	Total	C	N	O	S	0	0	0
			1123	718	194	207	4			
1	J	135	Total	C	N	O	S	0	0	0
			1056	675	183	194	4			
1	M	151	Total	C	N	O	S	0	0	0
			1163	740	203	215	5			
1	N	137	Total	C	N	O	S	0	0	0
			1075	686	186	198	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	expression tag	UNP Q72498
A	185	LYS	PHE	engineered mutation	UNP Q72498
B	50	GLY	-	expression tag	UNP Q72498
B	185	LYS	PHE	engineered mutation	UNP Q72498
E	50	GLY	-	expression tag	UNP Q72498
E	185	LYS	PHE	engineered mutation	UNP Q72498
F	50	GLY	-	expression tag	UNP Q72498
F	185	LYS	PHE	engineered mutation	UNP Q72498
I	50	GLY	-	expression tag	UNP Q72498
I	185	LYS	PHE	engineered mutation	UNP Q72498
J	50	GLY	-	expression tag	UNP Q72498
J	185	LYS	PHE	engineered mutation	UNP Q72498
M	50	GLY	-	expression tag	UNP Q72498

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Chain	Residue	Modelled	Actual	Comment	Reference
M	185	LYS	PHE	engineered mutation	UNP Q72498
N	50	GLY	-	expression tag	UNP Q72498
N	185	LYS	PHE	engineered mutation	UNP Q72498

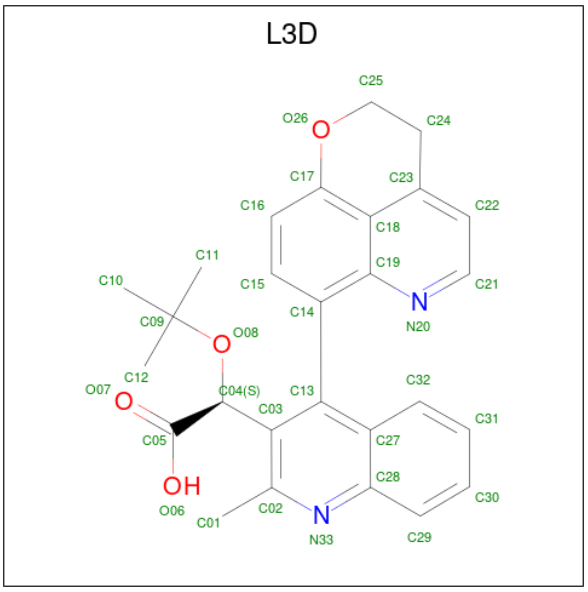
- Molecule 2 is a protein called Integrase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	46	Total	C	N	O	0	0	0
			389	253	73	63			
2	D	50	Total	C	N	O	0	0	0
			420	270	79	71			
2	G	49	Total	C	N	O	0	0	0
			410	265	76	69			
2	H	50	Total	C	N	O	0	0	0
			420	270	79	71			
2	K	46	Total	C	N	O	0	0	0
			385	252	70	63			
2	L	51	Total	C	N	O	0	0	0
			429	275	81	73			
2	O	48	Total	C	N	O	0	0	0
			404	262	75	67			
2	P	52	Total	C	N	O	0	0	0
			437	281	82	74			

There are 8 discrepancies between the modelled and reference sequences:

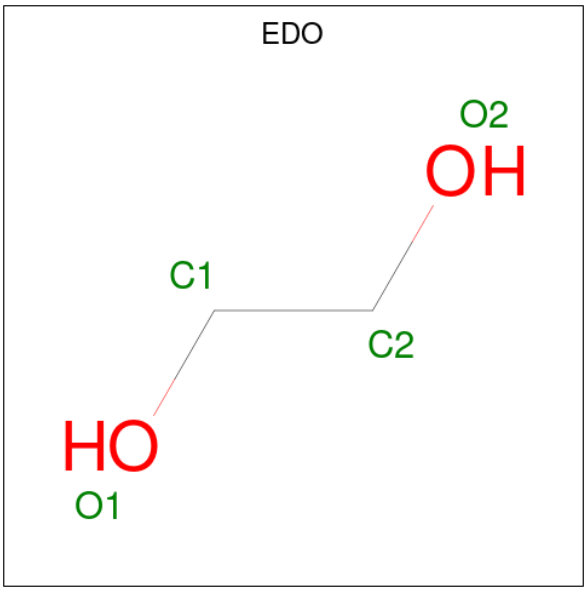
Chain	Residue	Modelled	Actual	Comment	Reference
C	219	GLY	-	expression tag	UNP Q72498
D	219	GLY	-	expression tag	UNP Q72498
G	219	GLY	-	expression tag	UNP Q72498
H	219	GLY	-	expression tag	UNP Q72498
K	219	GLY	-	expression tag	UNP Q72498
L	219	GLY	-	expression tag	UNP Q72498
O	219	GLY	-	expression tag	UNP Q72498
P	219	GLY	-	expression tag	UNP Q72498

- Molecule 3 is (2S)-tert-butoxy[4-(2,3-dihydropyrano[4,3,2-de]quinolin-7-yl)-2-methylquinolin-3-yl]acetic acid (three-letter code: L3D) (formula: $C_{27}H_{26}N_2O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 27 2 4	0	0
3	B	1	Total C N O 33 27 2 4	0	0
3	E	1	Total C N O 33 27 2 4	0	0
3	F	1	Total C N O 33 27 2 4	0	0
3	I	1	Total C N O 33 27 2 4	0	0
3	J	1	Total C N O 33 27 2 4	0	0
3	M	1	Total C N O 33 27 2 4	0	0
3	N	1	Total C N O 33 27 2 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	I	1	Total C O 4 2 2	0	0
4	J	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	K	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	L	1	Total C O 4 2 2	0	0
4	M	1	Total C O 4 2 2	0	0
4	N	1	Total C O 4 2 2	0	0
4	N	1	Total C O 4 2 2	0	0
4	O	1	Total C O 4 2 2	0	0
4	P	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total O 2 2	0	0
5	B	2	Total O 2 2	0	0
5	D	3	Total O 3 3	0	0
5	E	5	Total O 5 5	0	0
5	F	5	Total O 5 5	0	0
5	H	5	Total O 5 5	0	0

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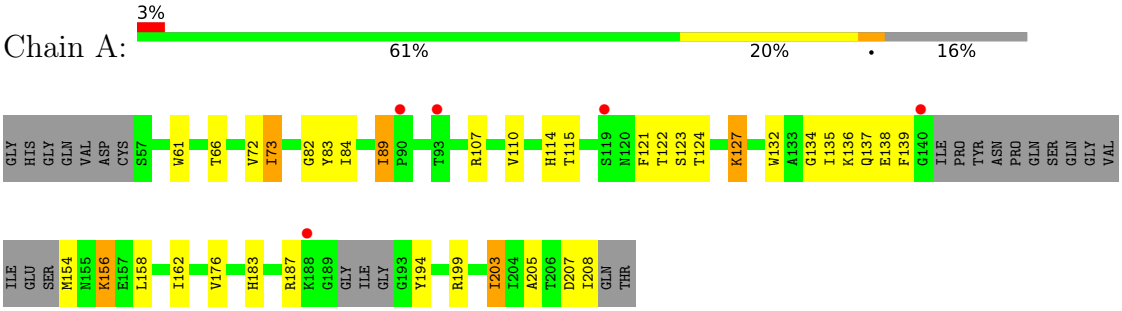
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	9	Total O 9 9	0	0
5	J	8	Total O 8 8	0	0
5	L	7	Total O 7 7	0	0
5	M	6	Total O 6 6	0	0
5	N	11	Total O 11 11	0	0
5	O	1	Total O 1 1	0	0
5	P	1	Total O 1 1	0	0

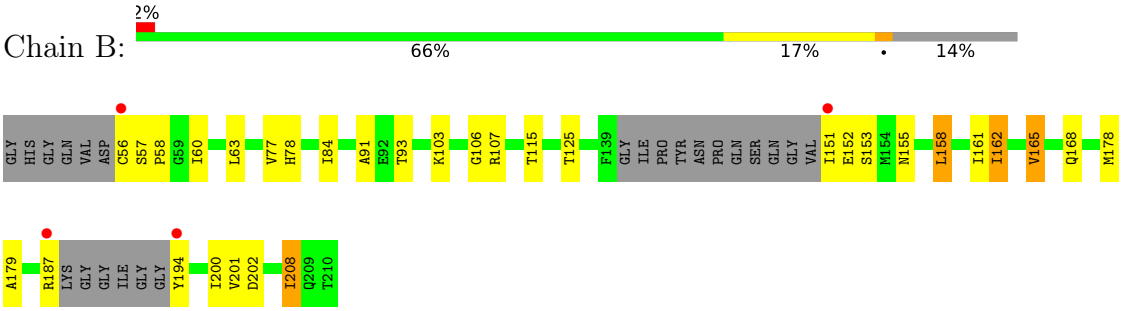
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

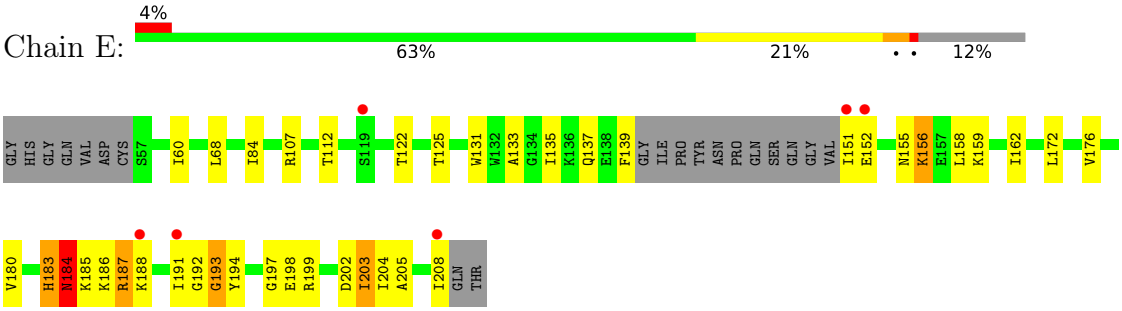
• Molecule 1: Integrase



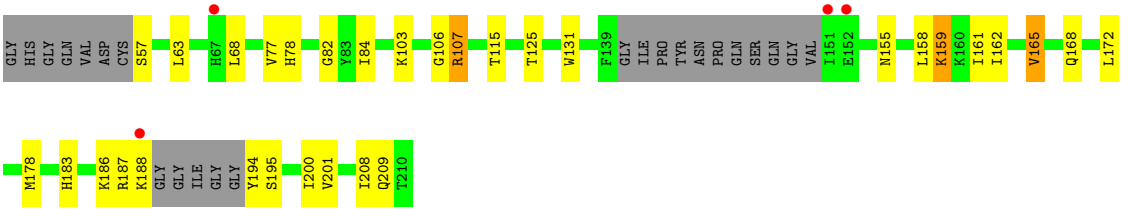
• Molecule 1: Integrase



• Molecule 1: Integrase

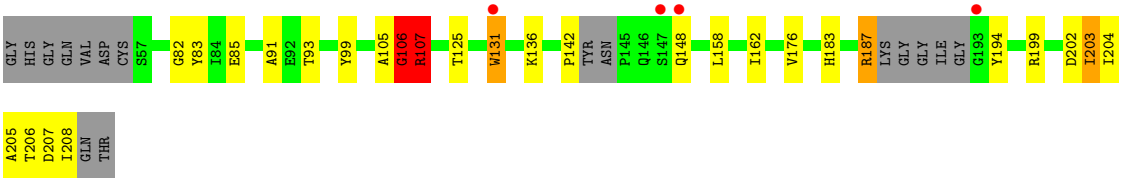


• Molecule 1: Integrase



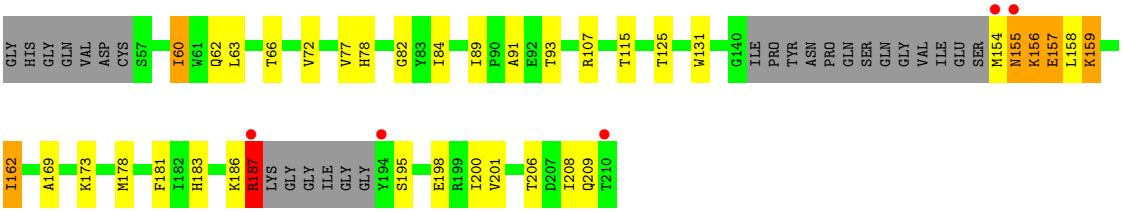
• Molecule 1: Integrase

Chain I:



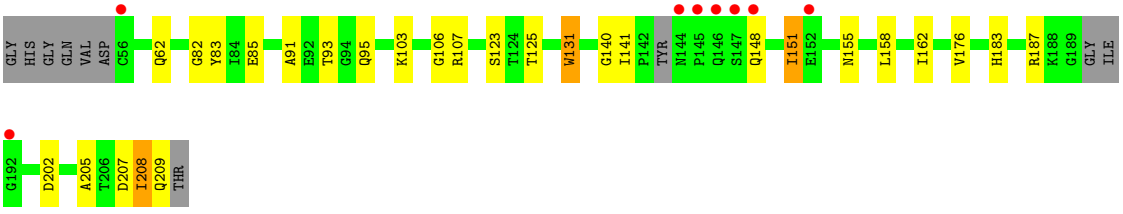
• Molecule 1: Integrase

Chain J:



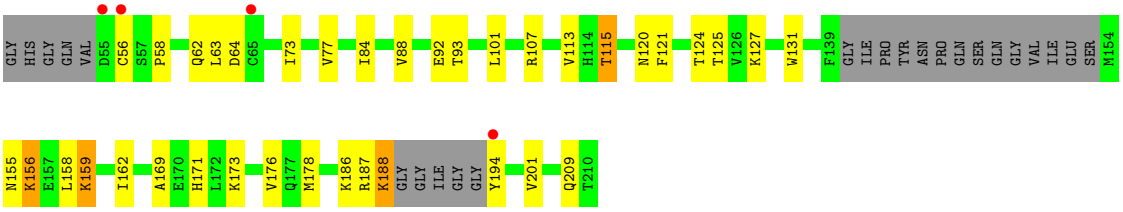
• Molecule 1: Integrase

Chain M:



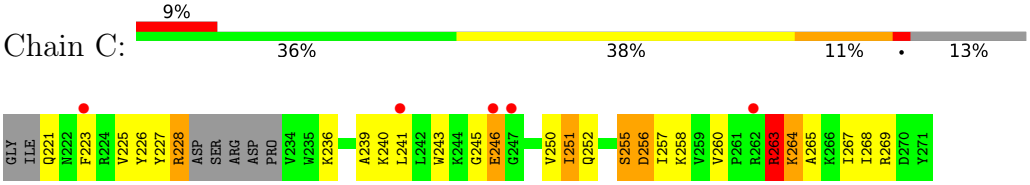
• Molecule 1: Integrase

Chain N:



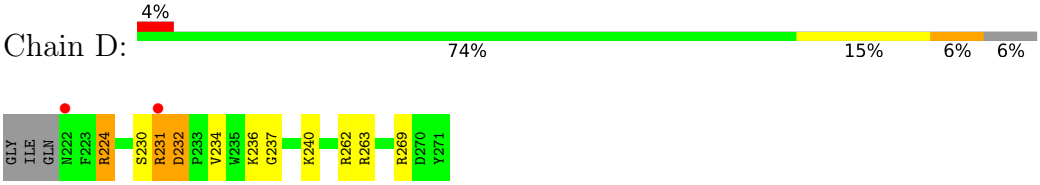
• Molecule 2: Integrase

Chain C:



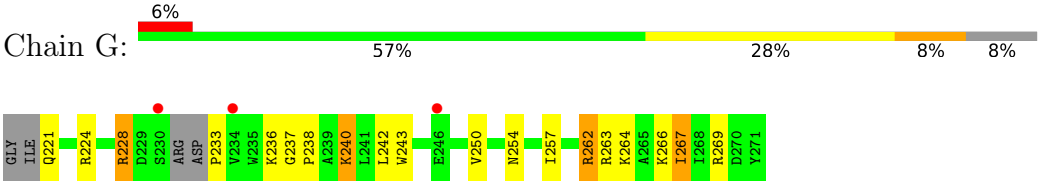
• Molecule 2: Integrase

Chain D:



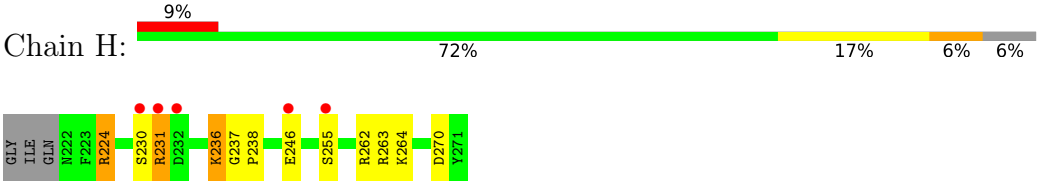
• Molecule 2: Integrase

Chain G:



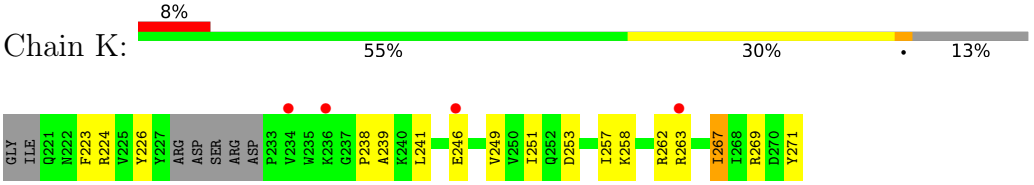
• Molecule 2: Integrase

Chain H:



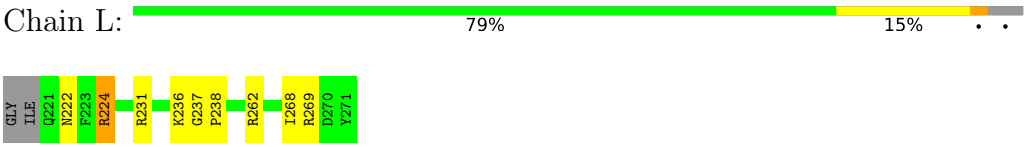
• Molecule 2: Integrase

Chain K:



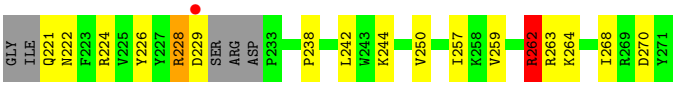
• Molecule 2: Integrase

Chain L:

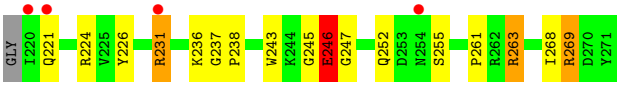


• Molecule 2: Integrase

Chain O:



• Molecule 2: Integrase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	181.51Å 116.51Å 112.80Å 90.00° 103.61° 90.00°	Depositor
Resolution (Å)	19.85 – 2.93 19.84 – 2.93	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.85-2.93) 90.7 (19.84-2.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.216 , 0.261 0.223 , 0.271	Depositor DCC
R_{free} test set	4441 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.9	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12460	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5211e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L3D, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.55	0/1076	0.69	0/1453
1	B	0.48	1/1101 (0.1%)	0.63	0/1488
1	E	0.48	0/1112	0.70	1/1503 (0.1%)
1	F	0.46	0/1104	0.63	0/1491
1	I	0.47	0/1145	0.66	2/1549 (0.1%)
1	J	0.49	0/1076	0.69	0/1454
1	M	0.48	0/1185	0.66	0/1602
1	N	0.47	0/1095	0.65	0/1479
2	C	0.46	0/397	0.82	1/531 (0.2%)
2	D	0.44	0/430	0.82	0/578
2	G	0.50	0/419	0.80	0/561
2	H	0.43	0/430	0.84	0/578
2	K	0.42	0/394	0.74	0/528
2	L	0.46	0/439	0.81	0/590
2	O	0.44	0/413	0.77	0/553
2	P	0.45	0/447	0.81	0/601
All	All	0.48	1/12263 (0.0%)	0.71	4/16539 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	1
1	F	0	1
1	I	0	1
1	J	0	2
1	M	0	2
2	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4
2	G	0	3
2	H	0	4
2	K	0	3
2	L	0	3
2	O	0	1
2	P	0	4
All	All	0	33

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	ILE	CG1-CD1	-5.78	1.10	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	184	ASN	N-CA-C	-7.60	90.48	111.00
1	I	106	GLY	N-CA-C	-6.08	97.90	113.10
1	I	107	ARG	N-CA-C	5.98	127.16	111.00
2	C	264	LYS	CB-CA-C	5.14	120.69	110.40

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Peptide
1	A	187	ARG	Sidechain
2	C	228	ARG	Sidechain
2	C	263	ARG	Sidechain
2	D	224	ARG	Sidechain
2	D	262	ARG	Sidechain
2	D	263	ARG	Sidechain
2	D	269	ARG	Sidechain
1	E	187	ARG	Sidechain
1	F	107	ARG	Sidechain
2	G	224	ARG	Sidechain
2	G	228	ARG	Sidechain
2	G	262	ARG	Sidechain
2	H	224	ARG	Sidechain
2	H	236	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	H	262	ARG	Sidechain
2	H	263	ARG	Sidechain
1	I	187	ARG	Sidechain
1	J	154	MET	Peptide
1	J	187	ARG	Sidechain
2	K	262	ARG	Sidechain
2	K	263	ARG	Sidechain
2	K	269	ARG	Sidechain
2	L	224	ARG	Sidechain
2	L	262	ARG	Sidechain
2	L	269	ARG	Sidechain
1	M	140	GLY	Peptide
1	M	187	ARG	Sidechain
2	O	262	ARG	Sidechain
2	P	224	ARG	Sidechain
2	P	231	ARG	Sidechain
2	P	263	ARG	Sidechain
2	P	269	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1056	0	1067	37	0
1	B	1081	0	1087	31	0
1	E	1091	0	1104	35	0
1	F	1084	0	1095	34	0
1	I	1123	0	1132	26	0
1	J	1056	0	1063	42	0
1	M	1163	0	1169	29	0
1	N	1075	0	1082	33	0
2	C	389	0	406	33	0
2	D	420	0	432	5	0
2	G	410	0	423	15	0
2	H	420	0	432	10	0
2	K	385	0	401	20	0
2	L	429	0	440	7	0
2	O	404	0	418	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	437	0	451	15	0
3	A	33	0	0	0	0
3	B	33	0	0	1	0
3	E	33	0	0	0	0
3	F	33	0	0	0	0
3	I	33	0	0	0	0
3	J	33	0	0	2	0
3	M	33	0	0	0	0
3	N	33	0	0	2	0
4	A	4	0	6	3	0
4	B	8	0	12	0	0
4	D	8	0	12	2	0
4	E	12	0	18	3	0
4	F	20	0	30	7	0
4	G	4	0	6	0	0
4	H	4	0	6	2	0
4	I	4	0	6	0	0
4	J	4	0	6	0	0
4	K	8	0	12	2	0
4	L	12	0	18	1	0
4	M	4	0	6	0	0
4	N	8	0	12	2	0
4	O	4	0	6	1	0
4	P	4	0	6	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	D	3	0	0	0	0
5	E	5	0	0	0	0
5	F	5	0	0	1	0
5	H	5	0	0	1	0
5	I	9	0	0	0	0
5	J	8	0	0	0	0
5	L	7	0	0	0	0
5	M	6	0	0	1	0
5	N	11	0	0	4	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
All	All	12460	0	12364	350	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (350) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:267:ILE:CD1	2:G:267:ILE:CG1	1.77	1.59
2:C:241:LEU:HA	2:C:251:ILE:HD11	1.29	1.11
1:M:107:ARG:HD3	1:N:107:ARG:HD3	1.40	1.03
1:A:107:ARG:HD3	1:B:107:ARG:HD3	1.43	0.99
1:J:155:ASN:HA	1:J:157:GLU:CD	1.81	0.99
1:A:121:PHE:O	1:A:127:LYS:NZ	1.97	0.97
1:I:107:ARG:HD3	1:J:107:ARG:HD3	1.46	0.96
1:E:197:GLY:O	4:E:304:EDO:H22	1.68	0.92
1:E:183:HIS:C	1:E:184:ASN:O	2.04	0.92
1:A:66:THR:HB	1:A:73:ILE:CD1	2.00	0.92
1:A:66:THR:HB	1:A:73:ILE:HD13	1.53	0.91
1:E:187:ARG:NH1	1:E:198:GLU:OE1	2.04	0.91
2:C:250:VAL:O	2:C:251:ILE:HD13	1.71	0.90
1:I:207:ASP:O	1:I:208:ILE:HB	1.73	0.88
1:A:110:VAL:O	1:A:135:ILE:CD1	2.24	0.85
1:N:115:THR:HG21	1:N:121:PHE:CD1	2.12	0.85
2:C:241:LEU:HA	2:C:251:ILE:CD1	2.07	0.84
2:C:228:ARG:HD3	2:C:264:LYS:HB2	1.58	0.84
2:C:228:ARG:HD3	2:C:264:LYS:CB	2.08	0.83
1:M:151:ILE:O	1:M:155:ASN:ND2	2.12	0.83
2:G:243:TRP:HB3	2:G:250:VAL:CG2	2.09	0.82
1:M:62:GLN:NE2	1:M:151:ILE:HD11	1.94	0.82
1:A:72:VAL:O	1:A:89:ILE:HD13	1.80	0.81
1:F:103:LYS:HA	4:F:501:EDO:H12	1.61	0.81
2:K:223:PHE:HB3	2:K:267:ILE:HD11	1.61	0.81
1:J:187:ARG:HG3	1:J:187:ARG:HH11	1.46	0.80
1:A:110:VAL:O	1:A:135:ILE:HD12	1.81	0.78
1:J:156:LYS:HA	1:J:159:LYS:HE2	1.64	0.78
1:J:155:ASN:OD1	1:J:159:LYS:NZ	2.16	0.78
2:C:228:ARG:CZ	2:C:264:LYS:HB2	2.13	0.77
2:G:240:LYS:HA	2:G:240:LYS:HE2	1.68	0.76
1:I:99:TYR:CZ	1:J:173:LYS:HG2	2.22	0.75
1:N:178:MET:HE1	3:N:301:L3D:C22	2.16	0.75
1:I:105:ALA:O	1:I:106:GLY:O	2.04	0.74
1:E:183:HIS:O	1:E:184:ASN:O	2.03	0.74
1:F:103:LYS:HA	4:F:501:EDO:C1	2.16	0.74
2:G:228:ARG:HB2	2:G:264:LYS:HD2	1.70	0.74
2:C:228:ARG:CD	2:C:264:LYS:HB2	2.17	0.74
1:I:205:ALA:HB2	1:J:201:VAL:HG12	1.71	0.73
2:K:257:ILE:O	2:K:258:LYS:HE2	1.90	0.72
2:K:258:LYS:HE2	2:K:258:LYS:HA	1.70	0.72
1:F:159:LYS:HA	1:F:162:ILE:HD12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:HG21	1:A:137:GLN:HE21	1.55	0.71
1:M:205:ALA:HB2	1:N:201:VAL:HG12	1.71	0.71
1:J:72:VAL:HG13	1:J:89:ILE:HG12	1.72	0.71
1:J:77:VAL:HG22	1:J:84:ILE:CD1	2.21	0.71
1:J:169:ALA:HB2	1:J:178:MET:HE3	1.73	0.71
1:N:88:VAL:HG21	1:N:173:LYS:HB3	1.72	0.70
1:A:84:ILE:HD13	1:A:183:HIS:CD2	2.26	0.70
1:J:178:MET:HE1	3:J:301:L3D:C22	2.21	0.70
2:G:243:TRP:HB3	2:G:250:VAL:HG22	1.73	0.69
1:N:169:ALA:HB2	1:N:178:MET:HE3	1.74	0.69
1:B:161:ILE:O	1:B:165:VAL:HG23	1.93	0.69
1:E:192:GLY:O	1:E:194:TYR:CD1	2.46	0.69
1:M:207:ASP:O	1:M:209:GLN:HG3	1.91	0.69
2:G:262:ARG:HG3	2:G:262:ARG:HH11	1.57	0.68
2:H:246:GLU:O	5:H:401:HOH:O	2.11	0.68
2:C:250:VAL:O	2:C:251:ILE:CD1	2.41	0.68
1:F:187:ARG:O	1:F:188:LYS:HB3	1.94	0.68
1:B:162:ILE:HD13	1:B:179:ALA:CB	2.24	0.67
2:C:225:VAL:HG21	2:C:251:ILE:HG12	1.76	0.67
1:F:161:ILE:O	1:F:165:VAL:HG23	1.94	0.67
1:F:68:LEU:HD13	1:F:159:LYS:HD2	1.77	0.67
1:F:77:VAL:HG22	1:F:84:ILE:CD1	2.25	0.67
1:J:187:ARG:HH11	1:J:187:ARG:CG	2.07	0.67
1:B:77:VAL:HG22	1:B:84:ILE:CD1	2.25	0.66
1:B:158:LEU:O	1:B:162:ILE:HG12	1.95	0.66
2:C:228:ARG:NE	2:C:264:LYS:HB2	2.11	0.66
1:A:72:VAL:HG23	1:A:89:ILE:HG12	1.78	0.66
2:C:252:GLN:HE21	2:C:255:SER:CA	2.08	0.65
2:O:262:ARG:HG3	2:O:262:ARG:HH11	1.61	0.65
2:H:230:SER:OG	2:H:231:ARG:HD3	1.96	0.64
1:F:158:LEU:O	1:F:162:ILE:HG13	1.97	0.64
1:N:77:VAL:HG22	1:N:84:ILE:CD1	2.28	0.64
1:N:171:HIS:ND1	5:N:402:HOH:O	2.30	0.64
1:J:155:ASN:C	1:J:157:GLU:H	2.00	0.63
1:N:124:THR:OG1	5:N:401:HOH:O	2.14	0.63
1:J:155:ASN:HA	1:J:157:GLU:OE2	1.96	0.63
1:N:178:MET:CE	3:N:301:L3D:C22	2.75	0.63
1:B:202:ASP:OD1	2:H:264:LYS:HE2	1.99	0.62
1:N:73:ILE:HG13	1:N:88:VAL:HG12	1.81	0.62
1:E:84:ILE:HD12	1:E:183:HIS:HD2	1.64	0.62
2:C:228:ARG:HD3	2:C:264:LYS:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:MET:CE	3:J:301:L3D:C22	2.77	0.62
1:N:92:GLU:HG2	1:N:120:ASN:HD22	1.64	0.62
1:B:151:ILE:CD1	1:B:153:SER:OG	2.47	0.62
4:F:501:EDO:C2	5:F:604:HOH:O	2.48	0.62
2:O:244:LYS:HD2	2:O:262:ARG:HH22	1.65	0.62
2:P:252:GLN:HE21	2:P:255:SER:HA	1.64	0.62
4:A:302:EDO:C1	1:B:106:GLY:HA3	2.30	0.62
2:C:252:GLN:NE2	2:C:255:SER:HA	2.14	0.62
1:N:77:VAL:HG22	1:N:84:ILE:HD13	1.82	0.61
1:A:194:TYR:CE2	1:B:208:ILE:HD11	2.36	0.61
1:N:63:LEU:HD13	1:N:113:VAL:HG13	1.81	0.61
2:P:226:TYR:OH	4:P:301:EDO:O2	2.12	0.61
1:E:180:VAL:HG11	4:F:501:EDO:H22	1.83	0.60
2:O:228:ARG:O	2:O:264:LYS:HE3	2.01	0.60
1:A:136:LYS:HD2	1:A:138:GLU:OE2	2.01	0.60
1:J:195:SER:OG	1:J:198:GLU:HG3	2.01	0.60
1:F:187:ARG:CZ	1:F:194:TYR:HB2	2.32	0.60
1:E:205:ALA:HB2	1:F:201:VAL:HG12	1.84	0.59
1:J:155:ASN:OD1	1:J:159:LYS:CE	2.50	0.59
1:F:187:ARG:O	1:F:188:LYS:CB	2.50	0.59
1:I:99:TYR:CE1	1:J:173:LYS:HG2	2.37	0.59
1:E:187:ARG:HH12	1:E:198:GLU:CD	2.05	0.59
1:N:187:ARG:HD3	1:N:194:TYR:HD2	1.68	0.59
2:H:231:ARG:HD3	2:H:231:ARG:H	1.68	0.59
2:C:227:TYR:HA	2:C:265:ALA:HA	1.85	0.58
1:I:207:ASP:O	1:I:208:ILE:CB	2.49	0.58
1:M:123:SER:HB2	5:M:401:HOH:O	2.03	0.58
1:E:84:ILE:HD12	1:E:183:HIS:CD2	2.39	0.58
2:P:252:GLN:NE2	2:P:255:SER:HA	2.17	0.58
2:C:252:GLN:HE21	2:C:255:SER:N	2.02	0.58
2:G:228:ARG:HB2	2:G:264:LYS:CD	2.33	0.58
1:J:72:VAL:HG13	1:J:89:ILE:CG1	2.34	0.58
1:B:187:ARG:HE	1:B:194:TYR:HD2	1.50	0.58
1:E:162:ILE:HD13	1:E:176:VAL:HG22	1.86	0.58
1:A:84:ILE:HD13	1:A:183:HIS:HD2	1.68	0.57
1:E:133:ALA:HB3	1:E:135:ILE:HD12	1.86	0.57
2:H:231:ARG:H	2:H:231:ARG:CD	2.17	0.57
1:F:187:ARG:NH1	1:F:194:TYR:HB2	2.19	0.57
1:J:155:ASN:OD1	1:J:156:LYS:N	2.37	0.57
1:E:107:ARG:HD3	1:F:107:ARG:CD	2.35	0.57
1:A:72:VAL:CG2	1:A:89:ILE:HG12	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ILE:C	1:B:208:ILE:HD13	2.24	0.57
2:O:250:VAL:HG22	2:O:259:VAL:HG12	1.86	0.57
4:A:302:EDO:H12	1:B:103:LYS:O	2.05	0.57
1:I:131:TRP:HB2	2:K:224:ARG:NH1	2.20	0.56
1:J:156:LYS:HA	1:J:159:LYS:CE	2.33	0.56
2:L:222:ASN:HD21	2:L:224:ARG:NH2	2.03	0.56
1:E:184:ASN:O	1:E:186:LYS:N	2.32	0.56
2:G:240:LYS:HA	2:G:240:LYS:CE	2.33	0.56
1:E:122:THR:HG22	1:E:139:PHE:CE2	2.41	0.56
2:L:222:ASN:ND2	2:L:224:ARG:NH2	2.54	0.55
2:L:222:ASN:ND2	2:L:224:ARG:HH21	2.04	0.55
1:A:115:THR:OG1	1:A:121:PHE:CG	2.57	0.55
2:D:231:ARG:O	2:D:232:ASP:HB2	2.06	0.55
2:P:268:ILE:HB	4:P:301:EDO:H21	1.89	0.55
1:A:122:THR:HG22	1:A:139:PHE:CE2	2.41	0.55
2:D:224:ARG:HB2	4:D:301:EDO:H21	1.87	0.55
1:M:131:TRP:HB2	2:O:224:ARG:NH1	2.23	0.54
2:C:225:VAL:HG21	2:C:251:ILE:CG1	2.36	0.54
1:I:131:TRP:CB	2:K:224:ARG:NH1	2.70	0.54
1:B:56:CYS:C	1:B:58:PRO:HD3	2.27	0.54
2:C:263:ARG:HG2	2:C:264:LYS:HD2	1.90	0.54
2:O:221:GLN:O	2:O:270:ASP:HB2	2.07	0.54
1:A:83:TYR:C	1:A:84:ILE:HD12	2.27	0.54
1:I:131:TRP:CE3	2:K:224:ARG:HD2	2.42	0.54
1:A:72:VAL:HG23	1:A:89:ILE:CD1	2.38	0.54
1:E:122:THR:HG22	1:E:139:PHE:HE2	1.72	0.54
4:A:302:EDO:H11	1:B:106:GLY:HA3	1.90	0.54
1:E:155:ASN:O	1:E:159:LYS:HD2	2.07	0.54
2:K:257:ILE:O	2:K:258:LYS:CE	2.56	0.54
1:A:124:THR:HA	1:A:127:LYS:HB2	1.89	0.53
1:N:131:TRP:NE1	2:P:238:PRO:HG3	2.24	0.53
2:C:221:GLN:HB3	2:C:223:PHE:CE1	2.43	0.53
2:C:223:PHE:CD2	2:C:267:ILE:HD11	2.43	0.53
1:B:57:SER:N	1:B:58:PRO:HD3	2.23	0.53
1:E:131:TRP:NE1	2:G:238:PRO:HG3	2.23	0.53
1:M:131:TRP:CB	2:O:224:ARG:NH1	2.71	0.53
1:N:115:THR:CG2	1:N:121:PHE:CD1	2.88	0.53
1:A:122:THR:HG22	1:A:139:PHE:HE2	1.73	0.53
2:K:239:ALA:CB	2:K:251:ILE:HD13	2.38	0.52
1:J:155:ASN:OD1	1:J:159:LYS:HE3	2.09	0.52
2:D:224:ARG:HD2	4:D:301:EDO:H22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:62:GLN:CG	1:M:151:ILE:HG13	2.39	0.52
1:N:56:CYS:C	1:N:58:PRO:HD2	2.30	0.52
1:M:202:ASP:OD1	1:N:209:GLN:NE2	2.41	0.51
1:E:158:LEU:O	1:E:162:ILE:HG13	2.11	0.51
1:A:205:ALA:HB2	1:B:201:VAL:HG12	1.92	0.51
1:M:62:GLN:HG3	1:M:151:ILE:CD1	2.40	0.51
1:M:106:GLY:HA3	4:N:303:EDO:C2	2.41	0.51
1:M:148:GLN:HA	1:M:151:ILE:CG2	2.40	0.51
1:A:162:ILE:HD13	1:A:176:VAL:HG22	1.93	0.51
2:C:252:GLN:HE21	2:C:255:SER:HA	1.70	0.51
1:M:148:GLN:HA	1:M:151:ILE:HG22	1.92	0.51
2:G:228:ARG:NH1	2:G:233:PRO:O	2.44	0.51
1:M:162:ILE:HD13	1:M:176:VAL:HG22	1.92	0.51
1:E:107:ARG:HD3	1:F:107:ARG:HD3	1.93	0.50
1:I:106:GLY:HA2	1:J:181:PHE:HD1	1.77	0.50
1:B:158:LEU:CD2	1:B:162:ILE:HD11	2.41	0.50
2:C:243:TRP:HB3	2:C:250:VAL:CG1	2.42	0.50
1:M:62:GLN:CD	1:M:151:ILE:HD11	2.30	0.50
2:C:228:ARG:HG2	2:C:228:ARG:HH11	1.77	0.50
1:N:155:ASN:O	1:N:159:LYS:HG2	2.11	0.49
2:O:228:ARG:O	2:O:229:ASP:HB2	2.11	0.49
1:J:187:ARG:CG	1:J:187:ARG:NH1	2.70	0.49
1:E:107:ARG:HD3	1:F:107:ARG:HD2	1.94	0.49
1:M:103:LYS:O	4:N:303:EDO:H21	2.12	0.49
2:K:271:TYR:OXT	4:K:501:EDO:H21	2.13	0.49
1:N:62:GLN:NE2	1:N:64:ASP:OD1	2.45	0.49
2:G:242:LEU:CD1	2:G:257:ILE:HD12	2.42	0.49
1:J:77:VAL:HG22	1:J:84:ILE:HD11	1.93	0.49
1:N:115:THR:HG21	1:N:121:PHE:CG	2.47	0.49
1:N:156:LYS:CE	1:N:156:LYS:H	2.24	0.49
2:P:226:TYR:HH	4:P:301:EDO:HO2	1.53	0.49
2:G:228:ARG:CB	2:G:264:LYS:HD2	2.39	0.49
2:O:242:LEU:CD1	2:O:257:ILE:HD12	2.43	0.48
1:I:162:ILE:HD13	1:I:176:VAL:HG22	1.95	0.48
1:J:66:THR:HG21	1:J:159:LYS:HD2	1.95	0.48
2:C:260:VAL:HG11	2:C:265:ALA:HB2	1.94	0.48
2:G:221:GLN:HB3	2:G:269:ARG:HD2	1.95	0.48
2:K:241:LEU:CD1	2:K:249:VAL:CG2	2.91	0.48
2:G:228:ARG:HB2	2:G:264:LYS:CE	2.44	0.48
1:I:131:TRP:HB2	2:K:224:ARG:HH12	1.76	0.48
1:B:57:SER:HB3	1:B:60:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:63:LEU:HB2	1:J:115:THR:HG22	1.96	0.48
1:B:158:LEU:O	1:B:158:LEU:HD22	2.13	0.48
1:F:107:ARG:HH21	4:F:506:EDO:H11	1.79	0.48
1:M:131:TRP:CG	2:O:224:ARG:NH1	2.82	0.48
1:B:152:GLU:HG2	1:B:155:ASN:HB3	1.96	0.47
1:N:162:ILE:HD13	1:N:176:VAL:HG22	1.95	0.47
1:A:158:LEU:O	1:A:162:ILE:HG13	2.14	0.47
2:C:239:ALA:HB1	2:C:251:ILE:HG23	1.96	0.47
1:N:88:VAL:HG21	1:N:173:LYS:CB	2.42	0.47
1:N:158:LEU:O	1:N:162:ILE:HG13	2.15	0.47
1:I:105:ALA:C	1:I:106:GLY:O	2.53	0.47
1:M:158:LEU:O	1:M:162:ILE:HG13	2.14	0.47
1:A:72:VAL:HG23	1:A:89:ILE:CG1	2.44	0.47
1:A:72:VAL:CG2	1:A:89:ILE:O	2.63	0.47
1:N:127:LYS:HD2	2:P:238:PRO:HD3	1.97	0.47
1:I:187:ARG:HH12	1:I:194:TYR:HD1	1.61	0.47
2:P:246:GLU:HG2	2:P:247:GLY:N	2.29	0.47
1:B:165:VAL:HG13	1:B:168:GLN:NE2	2.29	0.47
2:K:223:PHE:HB3	2:K:267:ILE:CD1	2.41	0.47
1:N:156:LYS:H	1:N:156:LYS:HE3	1.80	0.47
2:O:221:GLN:N	2:O:221:GLN:OE1	2.48	0.47
1:B:162:ILE:CD1	1:B:179:ALA:CB	2.92	0.47
1:F:165:VAL:HG13	1:F:168:GLN:NE2	2.30	0.47
1:B:77:VAL:HG22	1:B:84:ILE:HD11	1.96	0.46
2:O:262:ARG:HG2	2:O:263:ARG:NH1	2.30	0.46
1:E:198:GLU:HB3	1:F:208:ILE:HD12	1.96	0.46
1:A:72:VAL:HG23	1:A:89:ILE:O	2.16	0.46
1:A:115:THR:CG2	1:A:137:GLN:HE21	2.24	0.46
1:I:158:LEU:O	1:I:162:ILE:HG13	2.15	0.46
2:C:221:GLN:HA	2:C:269:ARG:HD3	1.98	0.46
2:C:257:ILE:C	2:C:258:LYS:HD3	2.36	0.46
1:F:106:GLY:O	4:F:504:EDO:H22	2.16	0.46
2:P:243:TRP:CH2	2:P:245:GLY:HA3	2.51	0.46
1:E:197:GLY:O	4:E:304:EDO:C2	2.52	0.46
1:E:60:ILE:CD1	1:E:112:THR:HB	2.46	0.45
1:N:188:LYS:HE3	1:N:194:TYR:HA	1.98	0.45
1:B:202:ASP:OD1	2:H:264:LYS:CE	2.64	0.45
2:K:258:LYS:HE2	2:K:258:LYS:CA	2.44	0.45
1:F:165:VAL:CG1	1:F:178:MET:CE	2.94	0.45
1:M:208:ILE:O	1:M:209:GLN:HB2	2.16	0.45
1:F:165:VAL:CG1	1:F:178:MET:HE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:MET:N	1:A:156:LYS:HZ2	2.15	0.45
3:B:301:L3D:C22	2:C:268:ILE:HG12	2.46	0.45
1:B:151:ILE:HD11	1:B:153:SER:OG	2.17	0.45
1:M:83:TYR:CE1	1:M:85:GLU:HG3	2.52	0.45
1:A:122:THR:HA	1:A:127:LYS:NZ	2.31	0.45
1:F:77:VAL:HG22	1:F:84:ILE:HD11	1.98	0.45
1:F:188:LYS:HD3	1:F:188:LYS:C	2.37	0.45
2:K:224:ARG:NH1	2:K:226:TYR:OH	2.50	0.45
1:M:131:TRP:HB2	2:O:224:ARG:HH12	1.80	0.45
2:C:226:TYR:HA	2:C:236:LYS:O	2.17	0.44
1:I:82:GLY:O	1:I:183:HIS:HE1	2.01	0.44
1:I:142:PRO:HD2	1:I:148:GLN:HE21	1.83	0.44
1:J:155:ASN:HA	1:J:157:GLU:CG	2.47	0.44
1:J:91:ALA:HB1	1:J:93:THR:HG23	2.00	0.44
1:J:158:LEU:O	1:J:162:ILE:HG13	2.18	0.44
1:M:62:GLN:HG3	1:M:151:ILE:HG13	2.00	0.44
1:A:199:ARG:O	1:A:203:ILE:HD13	2.18	0.44
1:B:78:HIS:CD2	1:B:200:ILE:HG13	2.53	0.44
1:F:78:HIS:CD2	1:F:200:ILE:HG13	2.53	0.44
1:B:63:LEU:HB2	1:B:115:THR:HG22	2.00	0.44
2:H:270:ASP:OD1	4:H:301:EDO:C1	2.66	0.44
2:K:224:ARG:NE	2:K:238:PRO:CB	2.81	0.44
2:O:224:ARG:NH1	2:O:226:TYR:OH	2.51	0.44
2:P:268:ILE:HB	4:P:301:EDO:C2	2.48	0.44
2:O:262:ARG:HH11	2:O:262:ARG:CG	2.28	0.43
1:J:60:ILE:N	1:J:60:ILE:CD1	2.80	0.43
1:A:132:TRP:CZ2	1:B:178:MET:HG2	2.54	0.43
1:E:194:TYR:CE1	4:E:302:EDO:H21	2.53	0.43
2:C:243:TRP:CH2	2:C:245:GLY:HA3	2.54	0.43
1:J:131:TRP:CE3	2:L:224:ARG:NH1	2.86	0.43
1:A:61:TRP:CD1	1:A:110:VAL:HG23	2.53	0.43
2:H:224:ARG:HD2	4:H:301:EDO:H12	2.01	0.43
1:J:78:HIS:CD2	1:J:200:ILE:HG13	2.54	0.43
2:K:224:ARG:NH2	2:K:238:PRO:HG3	2.34	0.43
2:O:224:ARG:NE	2:O:238:PRO:CB	2.81	0.43
2:O:268:ILE:HB	4:O:301:EDO:H12	2.00	0.43
1:A:137:GLN:HG2	1:A:139:PHE:CE1	2.53	0.43
1:E:137:GLN:HG2	1:E:139:PHE:CE1	2.53	0.43
1:E:204:ILE:HB	1:F:201:VAL:HG11	2.01	0.43
1:I:199:ARG:O	1:I:203:ILE:HD13	2.18	0.43
1:J:60:ILE:N	1:J:60:ILE:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ARG:O	1:E:203:ILE:HD13	2.18	0.43
1:F:63:LEU:HB2	1:F:115:THR:HG22	2.00	0.43
1:J:72:VAL:CG1	1:J:89:ILE:O	2.67	0.43
1:J:155:ASN:C	1:J:157:GLU:N	2.71	0.43
1:M:82:GLY:O	1:M:183:HIS:HE1	2.02	0.43
2:H:236:LYS:O	2:H:237:GLY:O	2.37	0.43
1:J:131:TRP:NE1	2:L:238:PRO:HG3	2.34	0.42
1:F:131:TRP:NE1	2:H:238:PRO:HG3	2.34	0.42
1:I:83:TYR:CE1	1:I:85:GLU:HG3	2.55	0.42
1:M:95:GLN:HE21	1:M:95:GLN:HB3	1.68	0.42
2:C:226:TYR:O	2:C:265:ALA:HA	2.19	0.42
1:I:202:ASP:OD1	1:J:209:GLN:NE2	2.52	0.42
1:J:155:ASN:CG	1:J:159:LYS:HZ1	2.22	0.42
2:L:268:ILE:HG22	4:L:501:EDO:H11	2.02	0.42
1:E:156:LYS:HA	1:E:159:LYS:CD	2.50	0.42
1:F:188:LYS:C	1:F:188:LYS:CD	2.88	0.42
2:K:271:TYR:OXT	4:K:501:EDO:C2	2.68	0.42
1:J:155:ASN:O	1:J:157:GLU:N	2.53	0.42
1:E:156:LYS:HA	1:E:159:LYS:HD3	2.01	0.42
1:E:192:GLY:O	1:E:193:GLY:C	2.57	0.42
1:F:68:LEU:CD1	1:F:159:LYS:HD2	2.49	0.42
2:K:267:ILE:O	2:K:267:ILE:CG2	2.67	0.42
2:P:252:GLN:O	2:P:252:GLN:HG2	2.20	0.42
2:C:251:ILE:HA	2:C:251:ILE:HD12	1.80	0.42
1:F:165:VAL:CG1	1:F:168:GLN:NE2	2.83	0.42
1:I:131:TRP:CG	2:K:224:ARG:NH1	2.88	0.42
2:K:239:ALA:HB1	2:K:251:ILE:HD13	2.01	0.42
1:M:141:ILE:HG12	1:M:148:GLN:HG3	2.02	0.42
1:B:162:ILE:CD1	1:B:179:ALA:HB3	2.50	0.41
2:D:236:LYS:O	2:D:237:GLY:O	2.38	0.41
1:F:82:GLY:O	1:F:183:HIS:HE1	2.03	0.41
2:P:236:LYS:O	2:P:237:GLY:O	2.37	0.41
1:A:107:ARG:CD	1:B:107:ARG:HD3	2.31	0.41
1:A:123:SER:O	1:A:127:LYS:HD2	2.20	0.41
1:F:68:LEU:HD23	1:F:172:LEU:HD11	2.03	0.41
1:I:204:ILE:O	1:I:207:ASP:O	2.38	0.41
1:J:206:THR:HG22	2:P:261:PRO:CG	2.51	0.41
2:L:236:LYS:O	2:L:237:GLY:O	2.38	0.41
1:N:156:LYS:CE	1:N:156:LYS:N	2.83	0.41
1:N:93:THR:HG22	5:N:405:HOH:O	2.21	0.41
2:C:252:GLN:HB2	2:C:257:ILE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:91:ALA:HB1	1:I:93:THR:HG23	2.02	0.41
1:A:82:GLY:O	1:A:84:ILE:CD1	2.68	0.41
1:A:122:THR:HA	1:A:127:LYS:HZ1	1.85	0.41
1:B:91:ALA:HB1	1:B:93:THR:HG23	2.02	0.41
2:C:245:GLY:O	2:C:246:GLU:C	2.59	0.41
1:F:103:LYS:HE3	4:F:506:EDO:H21	2.01	0.41
1:M:107:ARG:HD3	1:N:107:ARG:CD	2.30	0.41
2:G:236:LYS:O	2:G:237:GLY:O	2.39	0.41
2:P:221:GLN:HG2	2:P:269:ARG:HD2	2.03	0.41
1:I:206:THR:HG22	2:P:263:ARG:CD	2.51	0.40
1:M:131:TRP:CG	2:O:224:ARG:CZ	3.04	0.40
1:J:82:GLY:O	1:J:183:HIS:HE1	2.05	0.40
1:E:156:LYS:HD2	1:E:156:LYS:C	2.42	0.40
1:E:192:GLY:O	1:E:194:TYR:HD1	2.00	0.40
1:I:187:ARG:NH1	1:I:194:TYR:HD1	2.20	0.40
1:M:91:ALA:HB1	1:M:93:THR:HG23	2.03	0.40
1:N:173:LYS:NZ	5:N:403:HOH:O	2.50	0.40
2:D:240:LYS:HA	2:D:240:LYS:HD2	1.90	0.40
1:E:68:LEU:HD23	1:E:172:LEU:HD11	2.03	0.40
1:E:202:ASP:OD1	1:F:209:GLN:NE2	2.55	0.40
2:O:224:ARG:NH2	2:O:238:PRO:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	130/161 (81%)	126 (97%)	3 (2%)	1 (1%)	19 49
1	B	132/161 (82%)	128 (97%)	4 (3%)	0	100 100
1	E	137/161 (85%)	127 (93%)	6 (4%)	4 (3%)	4 16
1	F	132/161 (82%)	127 (96%)	5 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	139/161 (86%)	134 (96%)	3 (2%)	2 (1%)	11 34
1	J	129/161 (80%)	123 (95%)	4 (3%)	2 (2%)	9 30
1	M	145/161 (90%)	142 (98%)	2 (1%)	1 (1%)	22 52
1	N	131/161 (81%)	127 (97%)	4 (3%)	0	100 100
2	C	42/53 (79%)	32 (76%)	7 (17%)	3 (7%)	1 2
2	D	48/53 (91%)	42 (88%)	3 (6%)	3 (6%)	1 3
2	G	45/53 (85%)	42 (93%)	3 (7%)	0	100 100
2	H	48/53 (91%)	44 (92%)	4 (8%)	0	100 100
2	K	42/53 (79%)	40 (95%)	1 (2%)	1 (2%)	6 21
2	L	49/53 (92%)	45 (92%)	4 (8%)	0	100 100
2	O	44/53 (83%)	38 (86%)	5 (11%)	1 (2%)	6 22
2	P	50/53 (94%)	45 (90%)	4 (8%)	1 (2%)	7 25
All	All	1443/1712 (84%)	1362 (94%)	62 (4%)	19 (1%)	12 35

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
2	D	232	ASP
1	E	185	LYS
1	E	188	LYS
1	I	107	ARG
1	J	156	LYS
1	M	208	ILE
2	C	246	GLU
2	C	256	ASP
1	E	184	ASN
1	E	193	GLY
1	I	106	GLY
1	J	155	ASN
2	C	255	SER
2	D	230	SER
2	O	222	ASN
2	P	246	GLU
2	D	234	VAL
2	K	246	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	110/130 (85%)	103 (94%)	7 (6%)	17 43
1	B	115/130 (88%)	111 (96%)	4 (4%)	36 67
1	E	114/130 (88%)	106 (93%)	8 (7%)	15 39
1	F	115/130 (88%)	108 (94%)	7 (6%)	18 45
1	I	119/130 (92%)	115 (97%)	4 (3%)	37 68
1	J	111/130 (85%)	102 (92%)	9 (8%)	11 31
1	M	123/130 (95%)	120 (98%)	3 (2%)	49 77
1	N	114/130 (88%)	107 (94%)	7 (6%)	18 45
2	C	40/46 (87%)	36 (90%)	4 (10%)	7 22
2	D	44/46 (96%)	43 (98%)	1 (2%)	50 78
2	G	43/46 (94%)	38 (88%)	5 (12%)	5 16
2	H	44/46 (96%)	42 (96%)	2 (4%)	27 58
2	K	40/46 (87%)	38 (95%)	2 (5%)	24 54
2	L	45/46 (98%)	44 (98%)	1 (2%)	52 78
2	O	42/46 (91%)	40 (95%)	2 (5%)	25 56
2	P	46/46 (100%)	44 (96%)	2 (4%)	29 60
All	All	1265/1408 (90%)	1197 (95%)	68 (5%)	22 51

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	89	ILE
1	A	114	HIS
1	A	127	LYS
1	A	156	LYS
1	A	203	ILE
1	A	208	ILE
1	B	125	THR

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	165	VAL
1	B	208	ILE
2	C	240	LYS
2	C	251	ILE
2	C	256	ASP
2	C	263	ARG
2	D	231	ARG
1	E	125	THR
1	E	151	ILE
1	E	152	GLU
1	E	156	LYS
1	E	183	HIS
1	E	191	ILE
1	E	203	ILE
1	E	208	ILE
1	F	57	SER
1	F	125	THR
1	F	155	ASN
1	F	159	LYS
1	F	165	VAL
1	F	186	LYS
1	F	195	SER
2	G	240	LYS
2	G	254	ASN
2	G	263	ARG
2	G	266	LYS
2	G	267	ILE
2	H	231	ARG
2	H	255	SER
1	I	125	THR
1	I	131	TRP
1	I	136	LYS
1	I	203	ILE
1	J	60	ILE
1	J	62	GLN
1	J	125	THR
1	J	157	GLU
1	J	159	LYS
1	J	162	ILE
1	J	186	LYS
1	J	187	ARG

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Mol	Chain	Res	Type
1	J	208	ILE
2	K	253	ASP
2	K	267	ILE
2	L	231	ARG
1	M	125	THR
1	M	131	TRP
1	M	151	ILE
1	N	101	LEU
1	N	115	THR
1	N	125	THR
1	N	156	LYS
1	N	159	LYS
1	N	186	LYS
1	N	188	LYS
2	O	228	ARG
2	O	262	ARG
2	P	231	ARG
2	P	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	GLN
1	A	183	HIS
1	B	78	HIS
1	B	95	GLN
1	B	168	GLN
1	B	183	HIS
2	C	252	GLN
1	E	67	HIS
1	E	183	HIS
1	F	78	HIS
1	F	168	GLN
1	F	183	HIS
1	I	183	HIS
1	J	62	GLN
1	J	78	HIS
1	J	183	HIS
2	L	222	ASN
1	M	95	GLN
1	M	144	ASN
1	M	148	GLN

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Mol	Chain	Res	Type
1	M	155	ASN
1	M	183	HIS
1	N	155	ASN
2	P	252	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

35 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	L	501	-	3,3,3	0.12	0	2,2,2	0.23	0
3	L3D	N	301	-	36,37,37	1.06	3 (8%)	46,56,56	0.93	2 (4%)
4	EDO	G	301	-	3,3,3	0.09	0	2,2,2	0.29	0
4	EDO	E	303	-	3,3,3	0.11	0	2,2,2	0.27	0
4	EDO	E	302	-	3,3,3	0.04	0	2,2,2	0.33	0
3	L3D	B	301	-	36,37,37	0.81	1 (2%)	46,56,56	1.02	4 (8%)
4	EDO	H	301	-	3,3,3	0.21	0	2,2,2	0.50	0
4	EDO	O	301	-	3,3,3	0.10	0	2,2,2	0.15	0
4	EDO	F	501	-	3,3,3	0.34	0	2,2,2	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	D	301	-	3,3,3	0.12	0	2,2,2	0.53	0
3	L3D	E	301	-	36,37,37	0.94	4 (11%)	46,56,56	0.97	2 (4%)
4	EDO	F	505	-	3,3,3	0.12	0	2,2,2	0.19	0
3	L3D	F	502	-	36,37,37	0.81	1 (2%)	46,56,56	0.95	3 (6%)
4	EDO	A	302	-	3,3,3	0.39	0	2,2,2	0.68	0
4	EDO	F	504	-	3,3,3	0.24	0	2,2,2	0.74	0
3	L3D	J	301	-	36,37,37	1.16	3 (8%)	46,56,56	0.95	3 (6%)
4	EDO	F	506	-	3,3,3	0.22	0	2,2,2	0.42	0
4	EDO	B	303	-	3,3,3	0.13	0	2,2,2	0.17	0
3	L3D	M	301	-	36,37,37	0.83	1 (2%)	46,56,56	1.01	3 (6%)
4	EDO	E	304	-	3,3,3	0.17	0	2,2,2	0.61	0
3	L3D	I	301	-	36,37,37	0.95	3 (8%)	46,56,56	1.04	2 (4%)
4	EDO	N	302	-	3,3,3	0.32	0	2,2,2	0.47	0
4	EDO	N	303	-	3,3,3	0.33	0	2,2,2	0.58	0
3	L3D	A	301	-	36,37,37	0.97	3 (8%)	46,56,56	1.11	4 (8%)
4	EDO	P	301	-	3,3,3	0.12	0	2,2,2	0.16	0
4	EDO	B	302	-	3,3,3	0.29	0	2,2,2	0.38	0
4	EDO	I	302	-	3,3,3	0.14	0	2,2,2	0.24	0
4	EDO	J	302	-	3,3,3	0.14	0	2,2,2	0.27	0
4	EDO	L	502	-	3,3,3	0.13	0	2,2,2	0.19	0
4	EDO	K	502	-	3,3,3	0.10	0	2,2,2	0.16	0
4	EDO	L	503	-	3,3,3	0.19	0	2,2,2	0.33	0
4	EDO	M	302	-	3,3,3	0.17	0	2,2,2	0.36	0
4	EDO	D	302	-	3,3,3	0.16	0	2,2,2	0.23	0
4	EDO	K	501	-	3,3,3	0.10	0	2,2,2	0.34	0
4	EDO	F	503	-	3,3,3	0.25	0	2,2,2	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	L	501	-	-	1/1/1/1	-
3	L3D	N	301	-	-	3/16/23/23	0/4/5/5
4	EDO	G	301	-	-	1/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-
3	L3D	B	301	-	-	4/16/23/23	0/4/5/5
4	EDO	H	301	-	-	0/1/1/1	-
4	EDO	O	301	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	F	501	-	-	1/1/1/1	-
4	EDO	D	301	-	-	1/1/1/1	-
3	L3D	E	301	-	-	3/16/23/23	0/4/5/5
4	EDO	F	505	-	-	0/1/1/1	-
3	L3D	F	502	-	-	2/16/23/23	0/4/5/5
4	EDO	A	302	-	-	1/1/1/1	-
4	EDO	F	504	-	-	1/1/1/1	-
3	L3D	J	301	-	-	3/16/23/23	0/4/5/5
4	EDO	F	506	-	-	1/1/1/1	-
4	EDO	B	303	-	-	1/1/1/1	-
3	L3D	M	301	-	-	3/16/23/23	0/4/5/5
4	EDO	E	304	-	-	1/1/1/1	-
3	L3D	I	301	-	-	2/16/23/23	0/4/5/5
4	EDO	N	302	-	-	1/1/1/1	-
4	EDO	N	303	-	-	0/1/1/1	-
3	L3D	A	301	-	-	3/16/23/23	0/4/5/5
4	EDO	P	301	-	-	1/1/1/1	-
4	EDO	B	302	-	-	1/1/1/1	-
4	EDO	I	302	-	-	0/1/1/1	-
4	EDO	J	302	-	-	1/1/1/1	-
4	EDO	L	502	-	-	1/1/1/1	-
4	EDO	K	502	-	-	1/1/1/1	-
4	EDO	L	503	-	-	1/1/1/1	-
4	EDO	M	302	-	-	0/1/1/1	-
4	EDO	D	302	-	-	1/1/1/1	-
4	EDO	K	501	-	-	1/1/1/1	-
4	EDO	F	503	-	-	1/1/1/1	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	301	L3D	C14-C19	-5.00	1.35	1.43
3	N	301	L3D	C14-C19	-4.15	1.36	1.43
3	I	301	L3D	C14-C19	-3.33	1.38	1.43
3	E	301	L3D	C14-C19	-2.86	1.38	1.43
3	M	301	L3D	C14-C19	-2.70	1.39	1.43
3	A	301	L3D	C14-C19	-2.64	1.39	1.43
3	B	301	L3D	C14-C19	-2.56	1.39	1.43
3	A	301	L3D	O06-C05	-2.48	1.22	1.30
3	N	301	L3D	C23-C18	-2.41	1.38	1.43
3	A	301	L3D	O26-C17	2.36	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	502	L3D	C14-C19	-2.32	1.39	1.43
3	J	301	L3D	O06-C05	-2.32	1.22	1.30
3	E	301	L3D	O06-C05	-2.30	1.23	1.30
3	J	301	L3D	C23-C18	-2.15	1.39	1.43
3	E	301	L3D	O26-C17	2.13	1.40	1.37
3	N	301	L3D	O06-C05	-2.04	1.23	1.30
3	I	301	L3D	O07-C05	2.03	1.28	1.22
3	E	301	L3D	C23-C18	-2.01	1.39	1.43
3	I	301	L3D	C23-C18	-2.01	1.39	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	L3D	O26-C17-C18	4.17	122.52	118.51
3	I	301	L3D	O26-C17-C18	3.74	122.10	118.51
3	M	301	L3D	O26-C17-C18	3.70	122.06	118.51
3	E	301	L3D	O26-C17-C18	3.52	121.89	118.51
3	B	301	L3D	O26-C17-C18	3.43	121.81	118.51
3	J	301	L3D	O26-C17-C18	3.35	121.72	118.51
3	N	301	L3D	O26-C17-C18	3.23	121.61	118.51
3	F	502	L3D	O26-C17-C18	3.04	121.43	118.51
3	N	301	L3D	C17-C18-C19	2.48	120.57	115.18
3	A	301	L3D	C17-C18-C19	2.43	120.47	115.18
3	E	301	L3D	C17-C18-C19	2.42	120.44	115.18
3	B	301	L3D	C17-C18-C19	2.40	120.41	115.18
3	J	301	L3D	C17-C18-C19	2.39	120.40	115.18
3	F	502	L3D	C17-C18-C19	2.31	120.22	115.18
3	A	301	L3D	C14-C19-N20	2.27	120.88	118.77
3	M	301	L3D	C17-C18-C19	2.24	120.06	115.18
3	I	301	L3D	C17-C18-C19	2.24	120.06	115.18
3	B	301	L3D	O08-C09-C12	-2.21	99.74	108.21
3	F	502	L3D	C14-C19-N20	2.18	120.80	118.77
3	B	301	L3D	C14-C19-N20	2.16	120.78	118.77
3	J	301	L3D	C15-C14-C19	2.16	120.24	117.62
3	M	301	L3D	C14-C19-N20	2.02	120.65	118.77
3	A	301	L3D	O08-C09-C12	-2.00	100.54	108.21

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	301	L3D	C03-C04-C05-O06

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Mol	Chain	Res	Type	Atoms
3	M	301	L3D	C03-C04-C05-O06
3	N	301	L3D	C03-C04-C05-O06
3	N	301	L3D	C03-C04-C05-O07
3	J	301	L3D	C03-C04-C05-O07
3	B	301	L3D	C03-C04-C05-O06
3	E	301	L3D	C03-C04-C05-O06
3	E	301	L3D	C03-C04-C05-O07
3	M	301	L3D	C03-C04-C05-O07
4	D	302	EDO	O1-C1-C2-O2
4	E	304	EDO	O1-C1-C2-O2
4	G	301	EDO	O1-C1-C2-O2
4	J	302	EDO	O1-C1-C2-O2
4	K	502	EDO	O1-C1-C2-O2
4	L	501	EDO	O1-C1-C2-O2
4	N	302	EDO	O1-C1-C2-O2
4	P	301	EDO	O1-C1-C2-O2
3	B	301	L3D	C03-C04-C05-O07
3	F	502	L3D	C03-C04-C05-O07
3	A	301	L3D	C03-C04-C05-O06
3	A	301	L3D	C03-C04-C05-O07
3	F	502	L3D	C03-C04-C05-O06
3	I	301	L3D	C03-C04-C05-O07
4	F	501	EDO	O1-C1-C2-O2
4	F	504	EDO	O1-C1-C2-O2
3	B	301	L3D	C03-C13-C14-C15
4	D	301	EDO	O1-C1-C2-O2
4	F	506	EDO	O1-C1-C2-O2
4	K	501	EDO	O1-C1-C2-O2
3	I	301	L3D	C03-C04-C05-O06
4	L	502	EDO	O1-C1-C2-O2
4	L	503	EDO	O1-C1-C2-O2
4	B	302	EDO	O1-C1-C2-O2
3	A	301	L3D	C02-C03-C04-O08
3	E	301	L3D	C02-C03-C04-O08
3	J	301	L3D	C02-C03-C04-O08
3	M	301	L3D	C02-C03-C04-O08
3	N	301	L3D	C02-C03-C04-O08
4	A	302	EDO	O1-C1-C2-O2
4	B	303	EDO	O1-C1-C2-O2
4	F	503	EDO	O1-C1-C2-O2
3	B	301	L3D	C27-C13-C14-C15

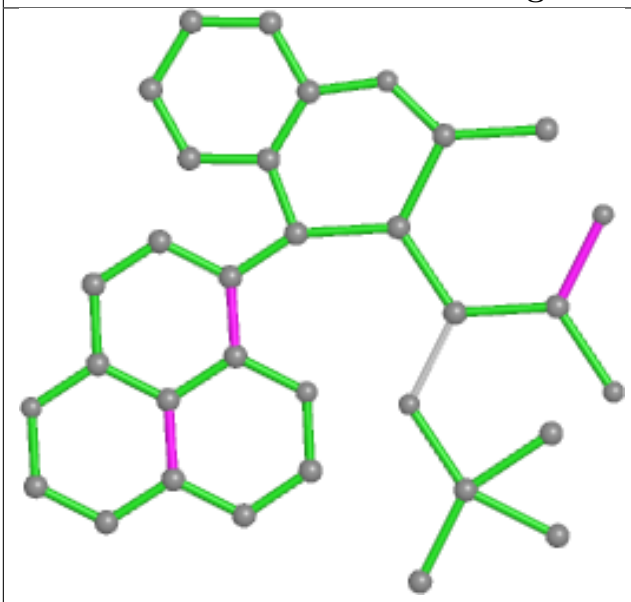
There are no ring outliers.

16 monomers are involved in 32 short contacts:

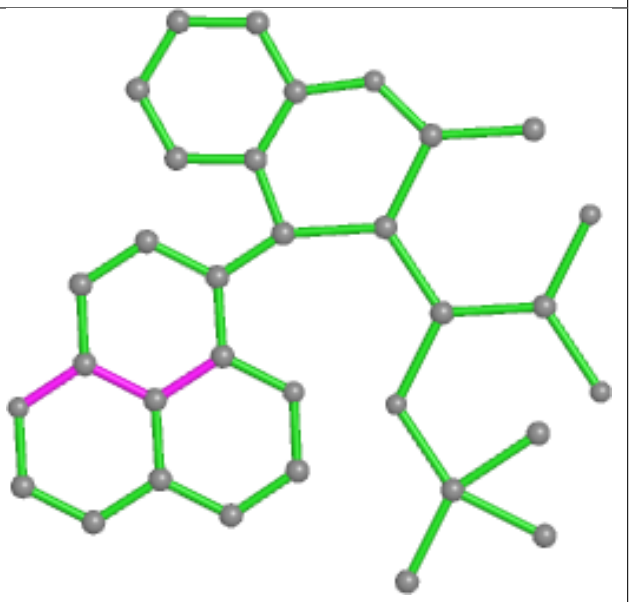
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	501	EDO	1	0
3	N	301	L3D	2	0
4	E	302	EDO	1	0
3	B	301	L3D	1	0
4	H	301	EDO	2	0
4	O	301	EDO	1	0
4	F	501	EDO	4	0
4	D	301	EDO	2	0
4	A	302	EDO	3	0
4	F	504	EDO	1	0
3	J	301	L3D	2	0
4	F	506	EDO	2	0
4	E	304	EDO	2	0
4	N	303	EDO	2	0
4	P	301	EDO	4	0
4	K	501	EDO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

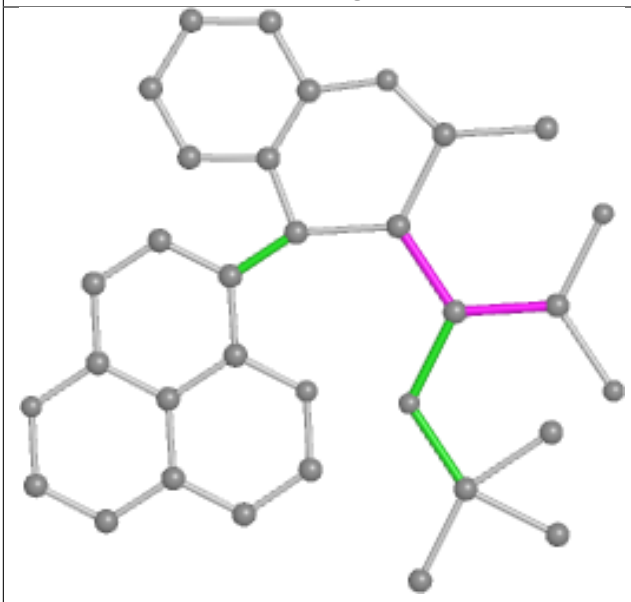
Ligand L3D N 301



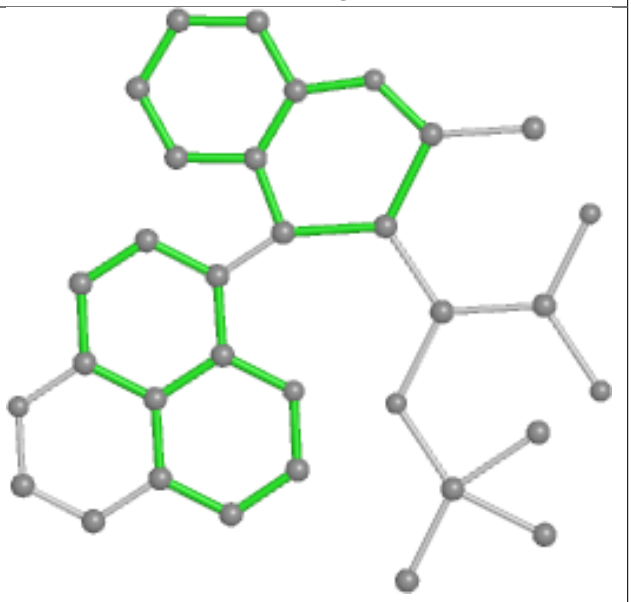
Bond lengths



Bond angles

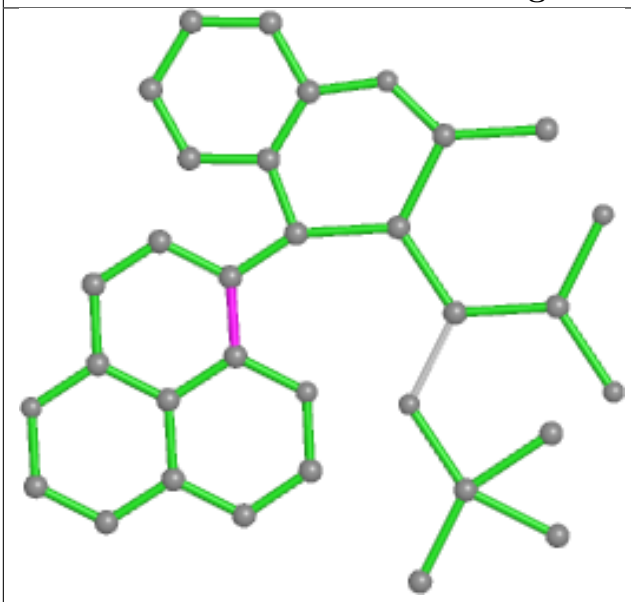


Torsions

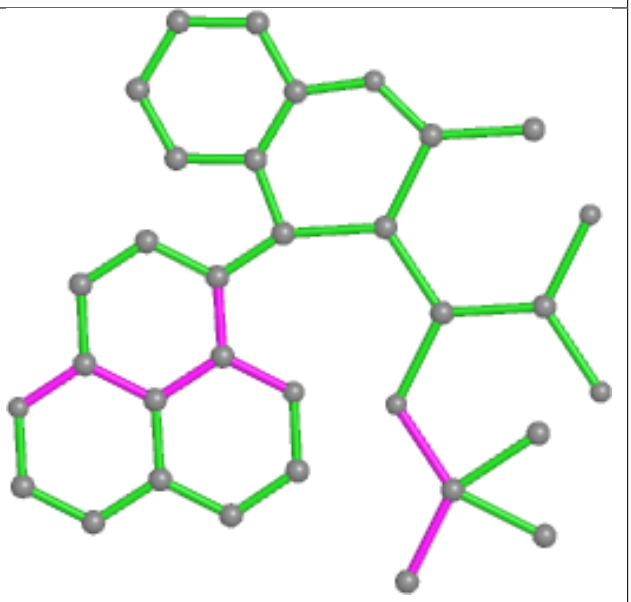


Rings

Ligand L3D B 301



Bond lengths



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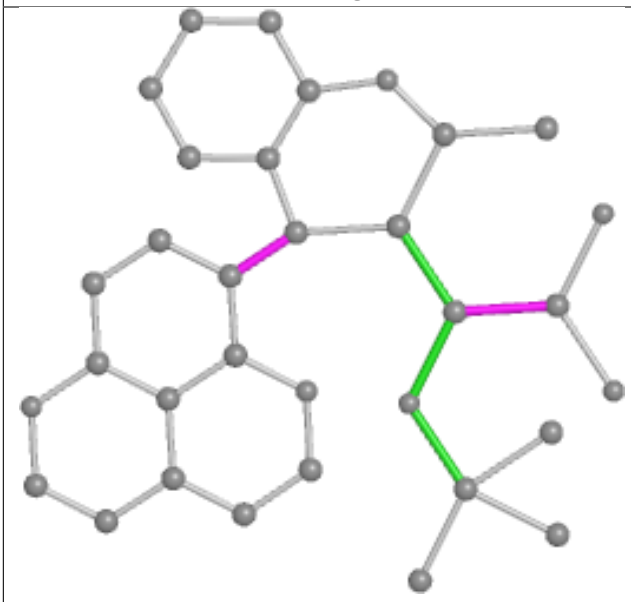
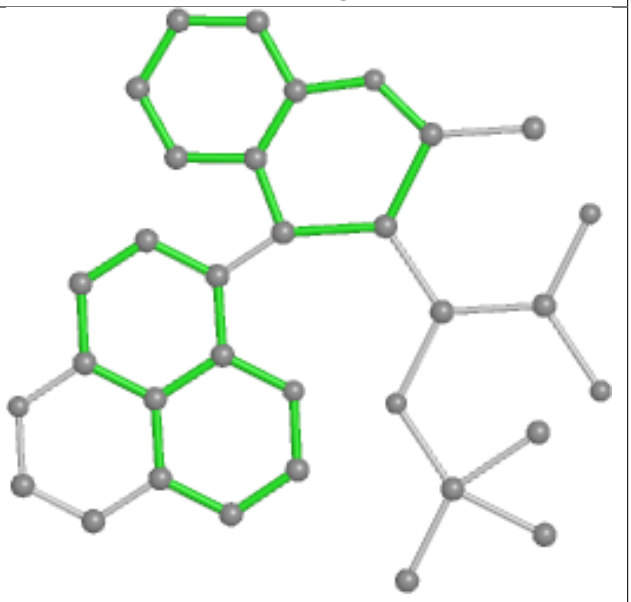
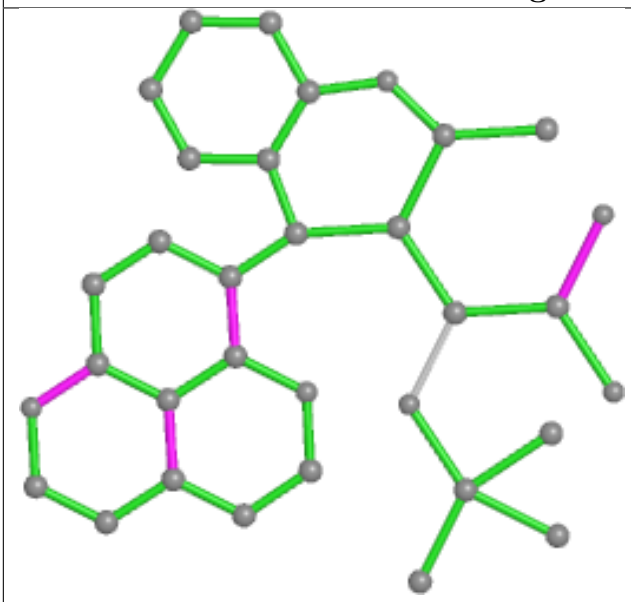


Torsions

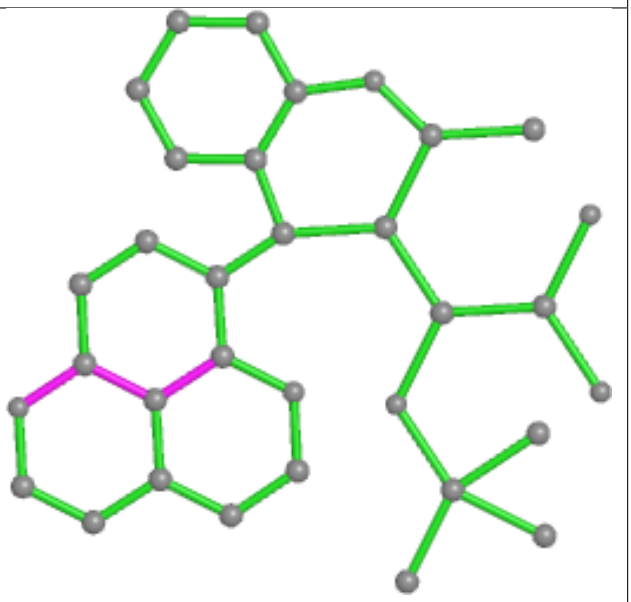


Rings

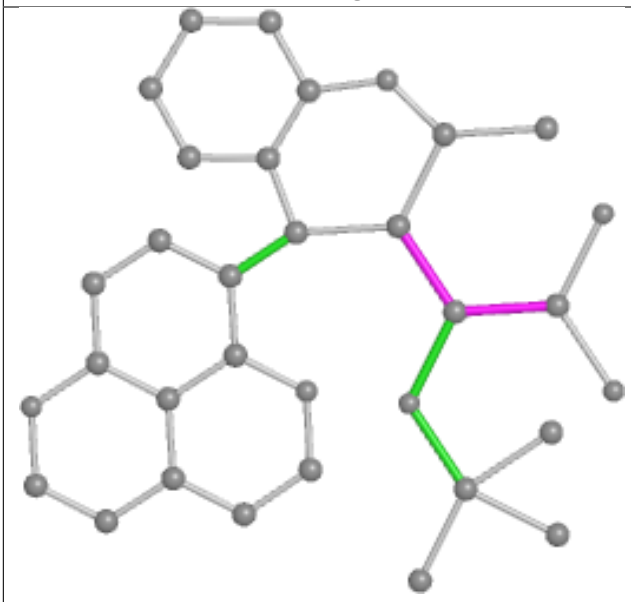
Ligand L3D E 301



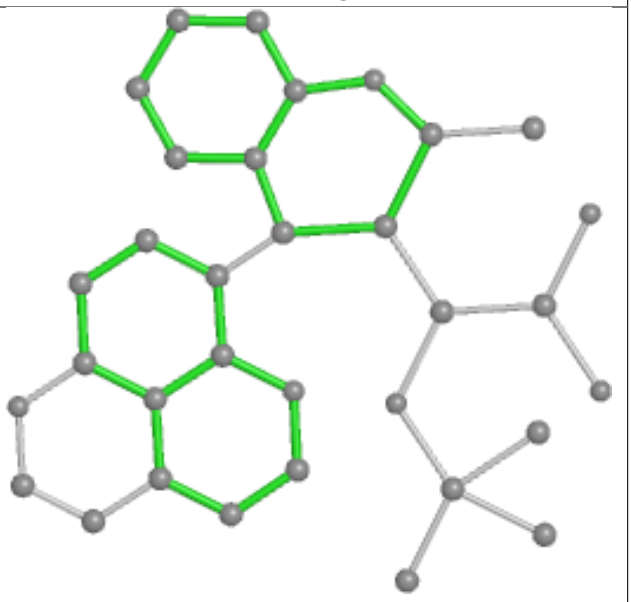
Bond lengths



Bond angles

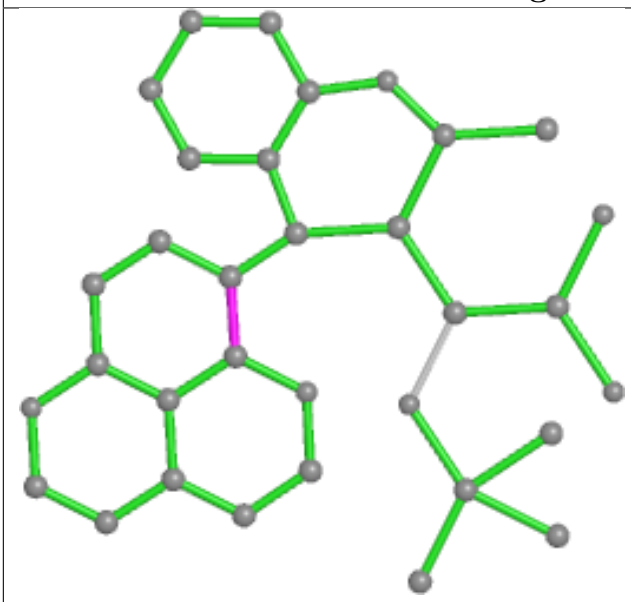


Torsions

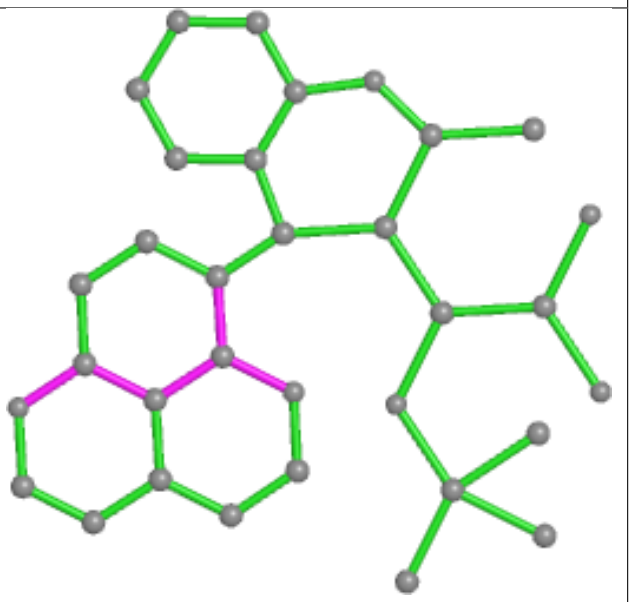


Rings

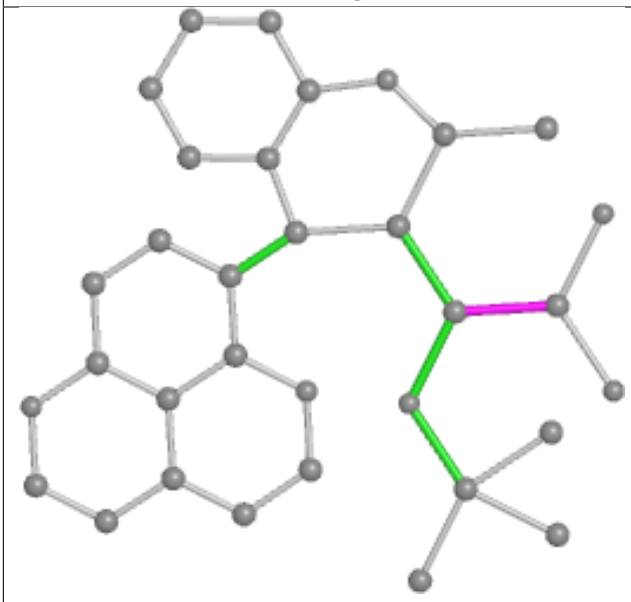
Ligand L3D F 502



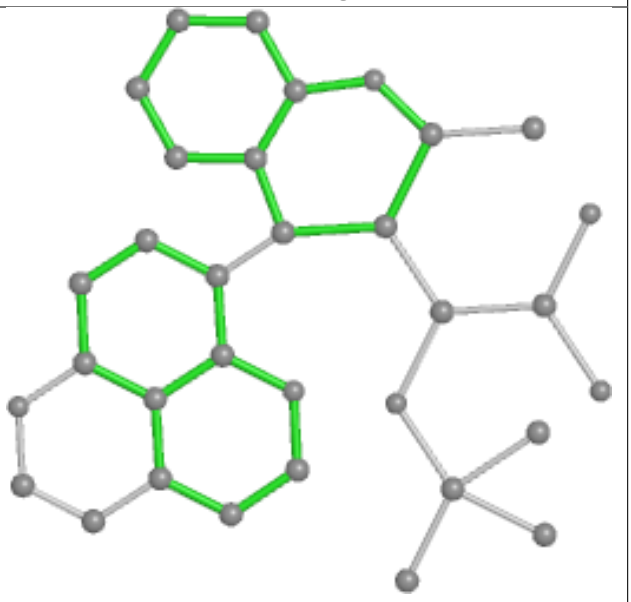
Bond lengths



Bond angles

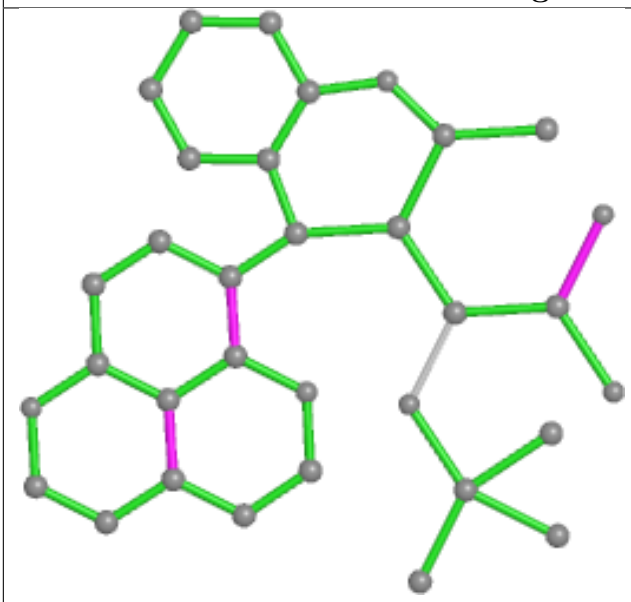


Torsions

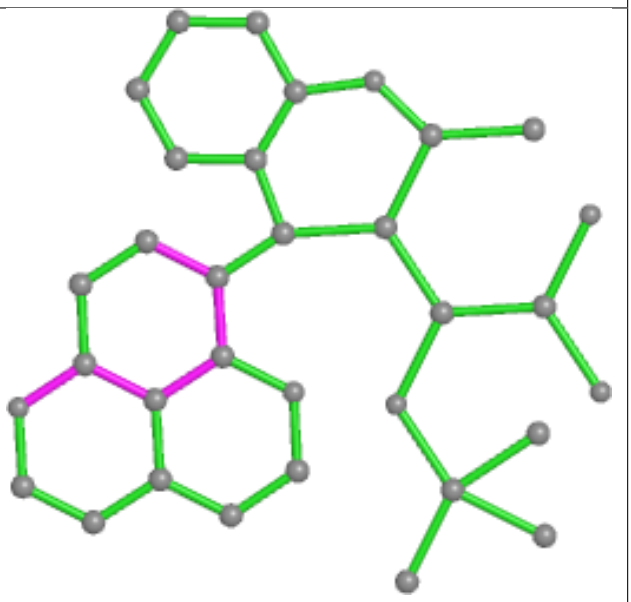


Rings

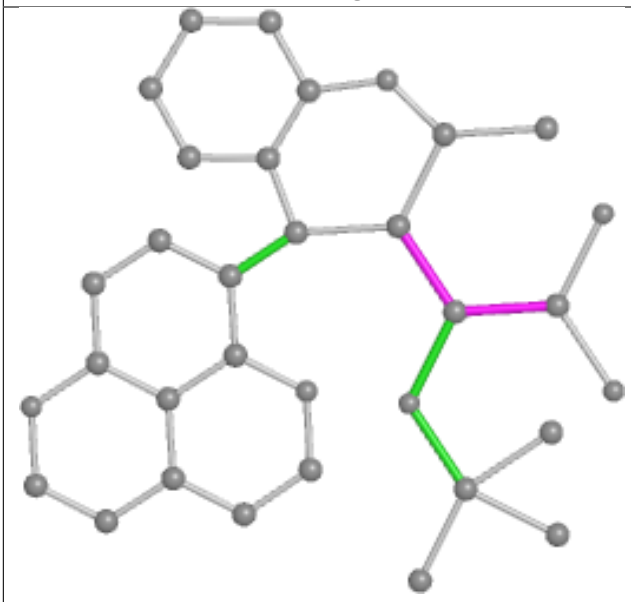
Ligand L3D J 301



Bond lengths



Bond angles



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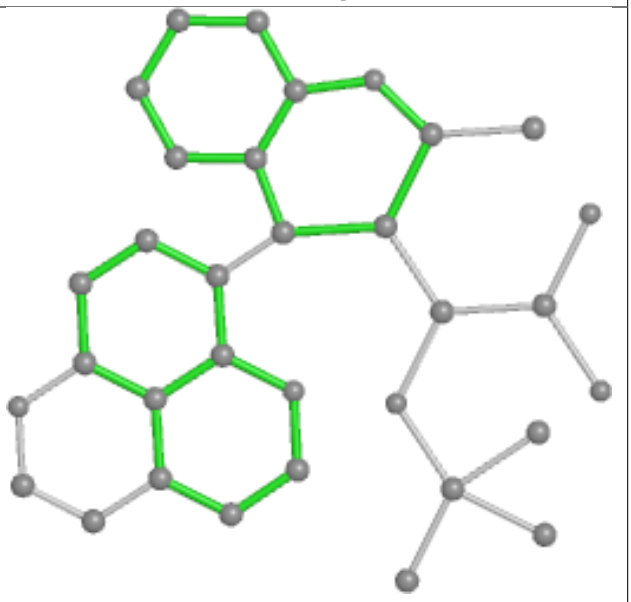
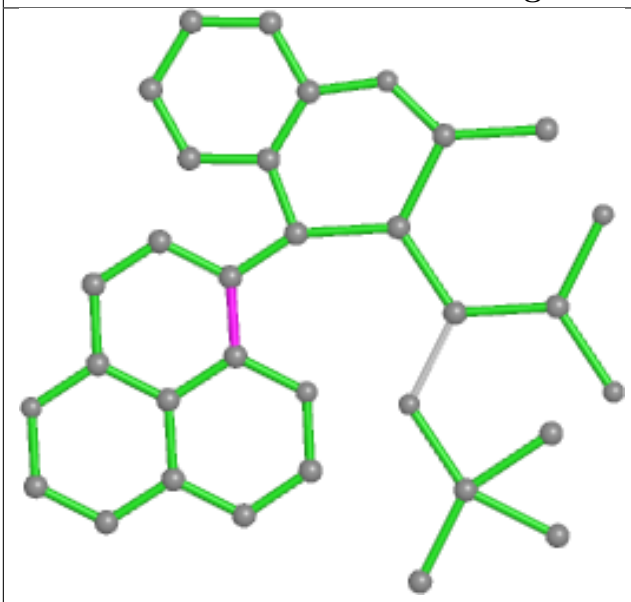


Rings

Ligand L3D M 301



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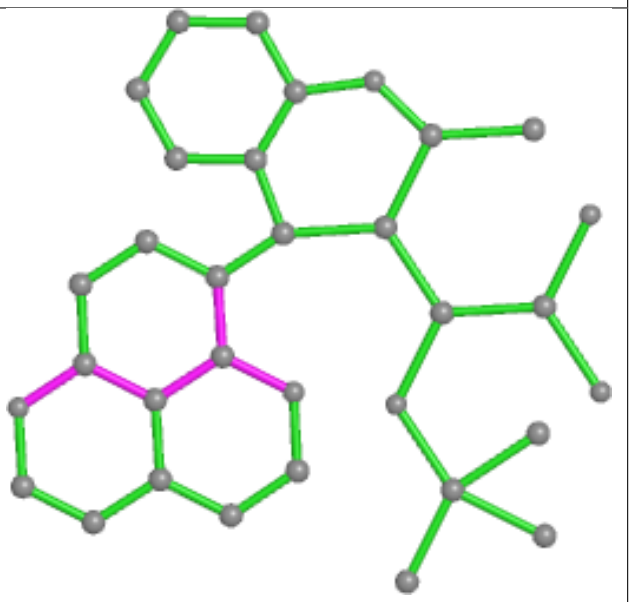
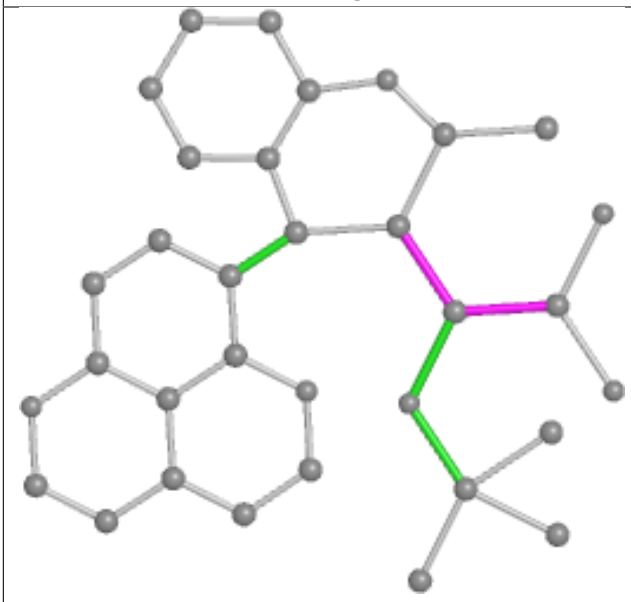
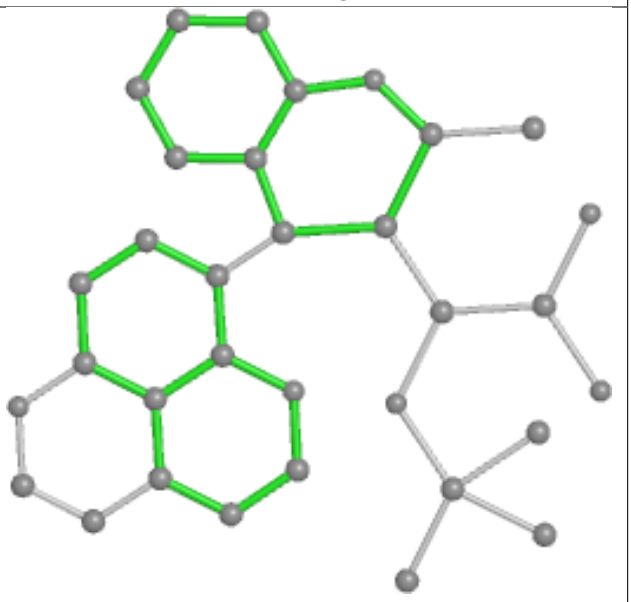


Bond angles

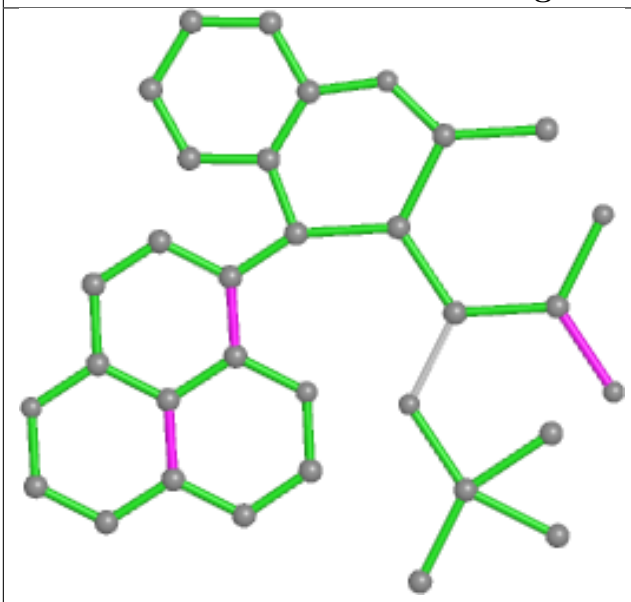


Torsions

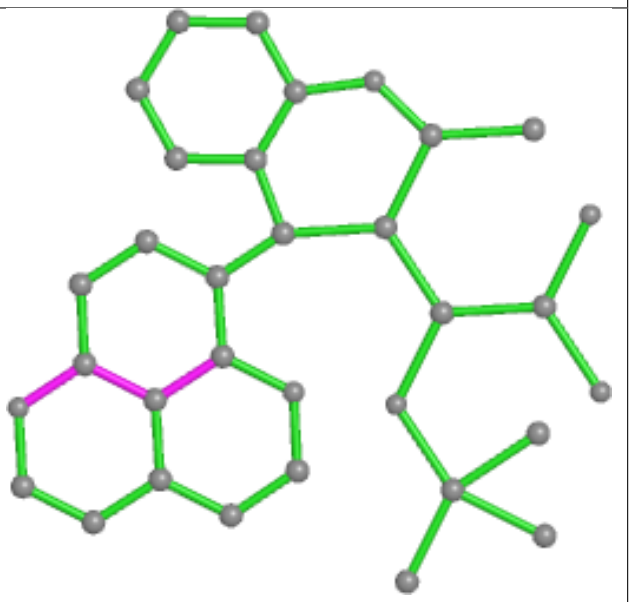


Rings

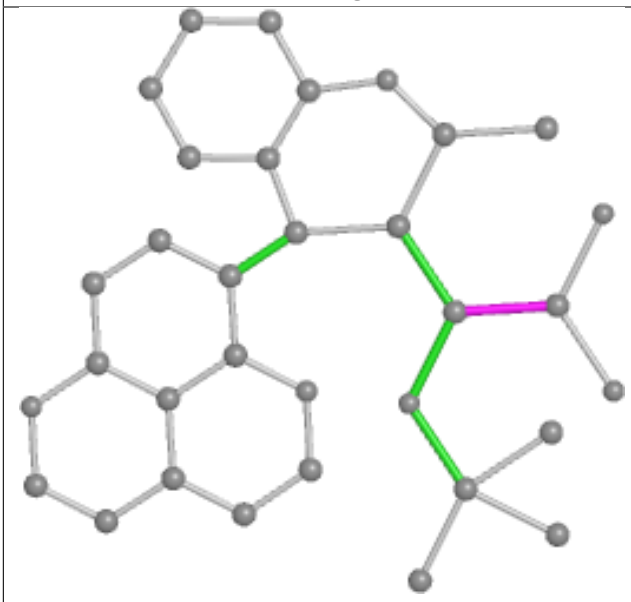
Ligand L3D I 301



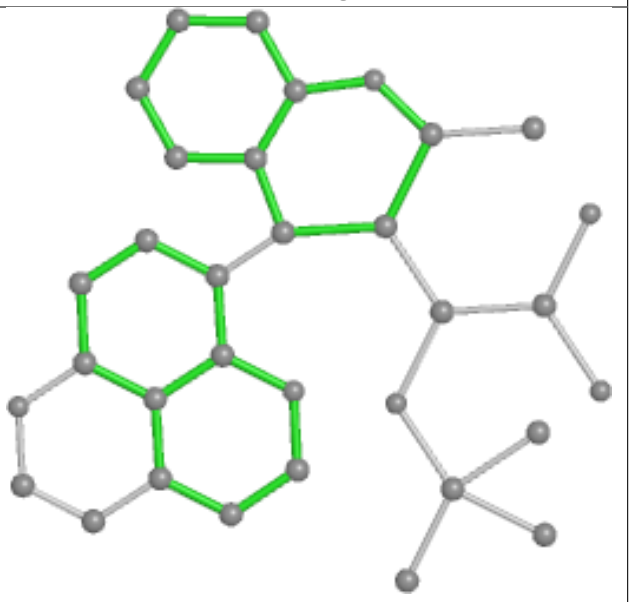
Bond lengths



Bond angles

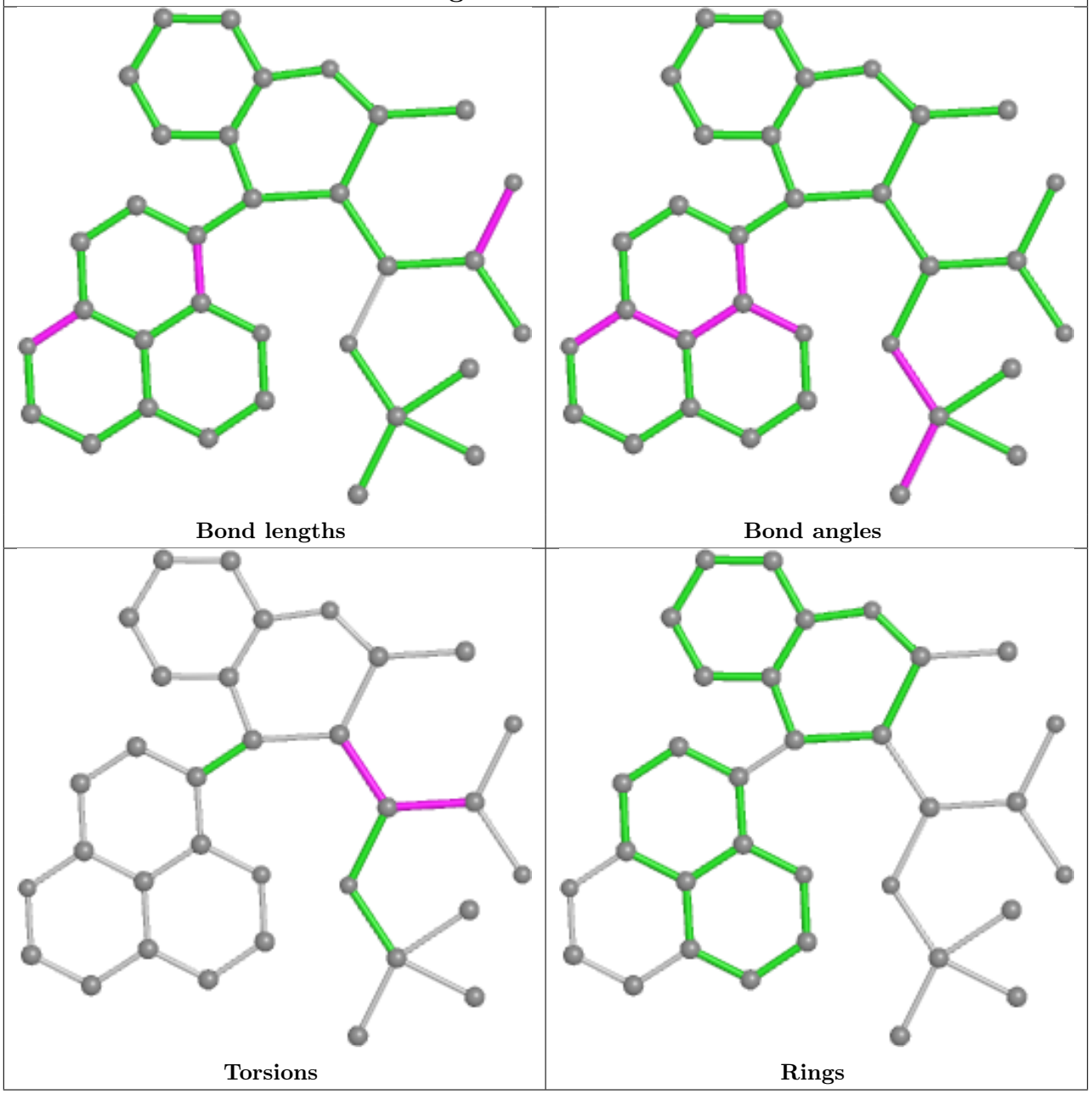


Torsions



Rings

Ligand L3D A 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	136/161 (84%)	0.05	5 (3%) 41 40	46, 89, 128, 168	0
1	B	138/161 (85%)	-0.10	4 (2%) 51 51	39, 77, 121, 134	0
1	E	141/161 (87%)	-0.18	6 (4%) 35 34	36, 69, 114, 141	0
1	F	138/161 (85%)	-0.31	4 (2%) 51 51	31, 63, 105, 138	0
1	I	145/161 (90%)	-0.24	4 (2%) 53 53	26, 62, 102, 125	0
1	J	135/161 (83%)	-0.28	5 (3%) 41 40	32, 69, 110, 158	0
1	M	151/161 (93%)	-0.24	8 (5%) 26 25	25, 58, 104, 127	0
1	N	137/161 (85%)	-0.18	4 (2%) 51 51	32, 66, 105, 152	0
2	C	46/53 (86%)	0.84	5 (10%) 5 5	108, 132, 150, 153	0
2	D	50/53 (94%)	-0.07	2 (4%) 38 37	37, 63, 117, 153	0
2	G	49/53 (92%)	0.62	3 (6%) 21 19	93, 107, 131, 136	0
2	H	50/53 (94%)	0.09	5 (10%) 7 6	39, 70, 131, 139	0
2	K	46/53 (86%)	0.42	4 (8%) 10 8	90, 103, 126, 141	0
2	L	51/53 (96%)	-0.14	0 100 100	39, 57, 105, 135	0
2	O	48/53 (90%)	0.40	1 (2%) 63 64	70, 96, 117, 131	0
2	P	52/53 (98%)	0.15	4 (7%) 13 11	40, 62, 119, 153	0
All	All	1513/1712 (88%)	-0.07	64 (4%) 36 35	25, 71, 127, 168	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	56	CYS	6.0
1	I	147	SER	5.4
1	B	56	CYS	4.8
1	J	194	TYR	4.4
2	G	230	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	151	ILE	4.0
1	B	151	ILE	4.0
2	H	231	ARG	4.0
1	M	147	SER	3.9
2	P	221	GLN	3.8
1	B	194	TYR	3.8
2	C	241	LEU	3.7
2	O	229	ASP	3.6
1	A	188	LYS	3.4
1	M	56	CYS	3.4
2	P	220	ILE	3.4
2	C	262	ARG	3.4
2	C	223	PHE	3.4
1	E	208	ILE	3.3
1	N	55	ASP	3.2
2	H	230	SER	3.2
2	G	234	VAL	3.1
2	P	231	ARG	3.1
1	E	119	SER	3.0
1	E	152	GLU	3.0
1	I	148	GLN	2.9
1	E	191	ILE	2.9
2	K	236	LYS	2.9
1	M	192	GLY	2.8
1	N	194	TYR	2.8
1	E	188	LYS	2.7
2	C	247	GLY	2.7
2	D	231	ARG	2.7
2	P	254	ASN	2.7
1	A	140	GLY	2.7
1	F	152	GLU	2.6
1	F	188	LYS	2.5
2	C	246	GLU	2.4
1	A	93	THR	2.4
1	J	210	THR	2.4
1	M	146	GLN	2.4
1	M	144	ASN	2.4
1	M	152	GLU	2.4
2	H	232	ASP	2.4
2	K	234	VAL	2.3
1	J	154	MET	2.3
1	A	119	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	246	GLU	2.3
2	K	246	GLU	2.3
1	M	145	PRO	2.3
1	J	155	ASN	2.3
2	K	263	ARG	2.2
2	D	222	ASN	2.2
2	H	255	SER	2.2
2	G	246	GLU	2.2
1	A	90	PRO	2.2
1	N	65	CYS	2.2
1	F	67	HIS	2.2
1	M	148	GLN	2.2
1	J	187	ARG	2.1
1	F	151	ILE	2.0
1	I	193	GLY	2.0
1	B	187	ARG	2.0
1	I	131	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	B	303	4/4	0.68	0.23	69,75,75,80	0
4	EDO	M	302	4/4	0.75	0.34	71,87,92,98	0
4	EDO	K	502	4/4	0.78	0.41	79,106,116,132	0
4	EDO	E	302	4/4	0.78	0.60	84,99,108,118	0
4	EDO	D	302	4/4	0.81	0.28	71,72,75,81	0
4	EDO	B	302	4/4	0.84	0.28	52,63,78,86	0

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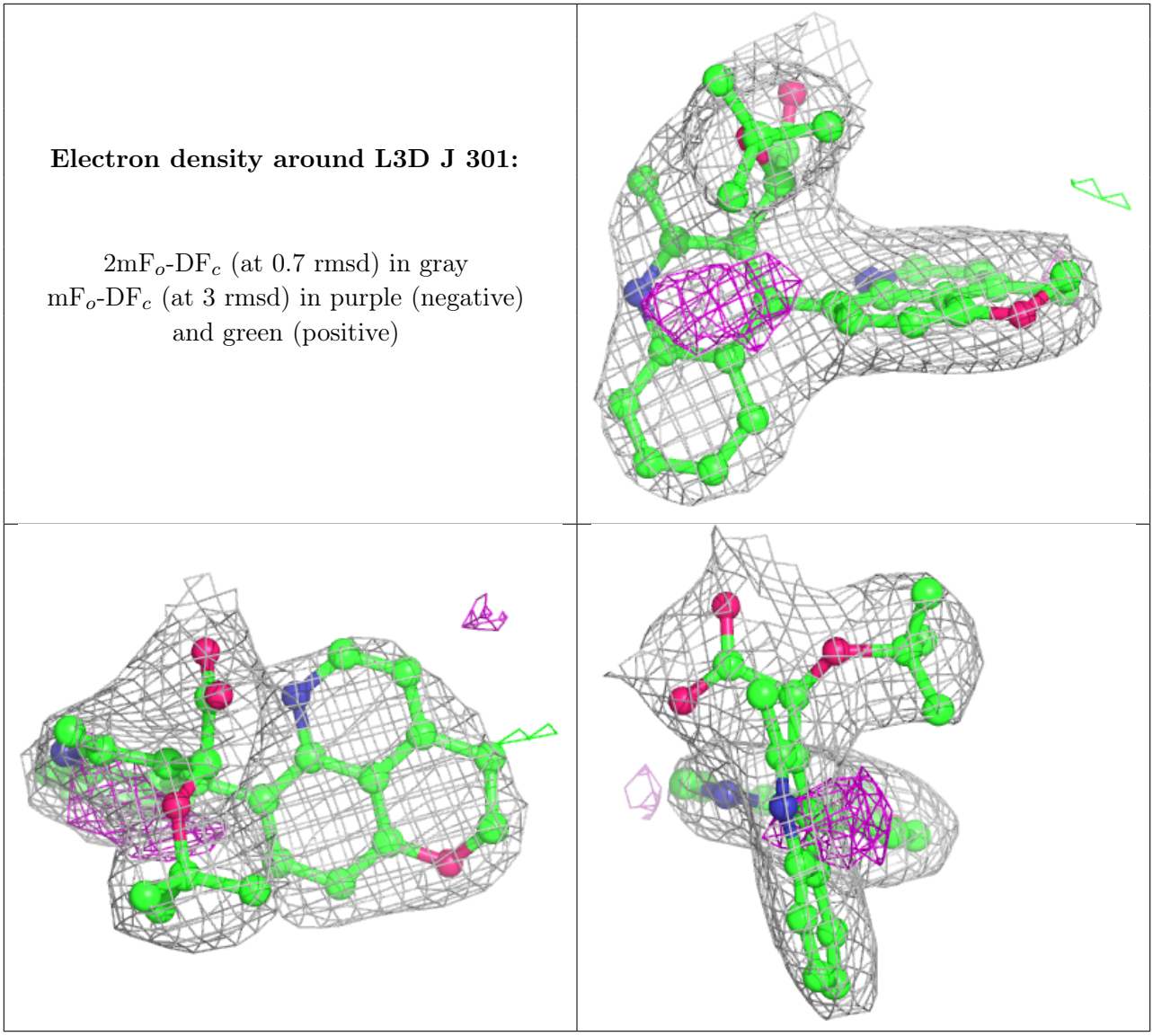
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	K	501	4/4	0.84	0.30	64,85,85,87	0
4	EDO	F	505	4/4	0.85	0.17	66,67,70,75	0
4	EDO	I	302	4/4	0.86	0.31	96,97,108,115	0
4	EDO	G	301	4/4	0.86	0.42	141,145,153,164	0
4	EDO	L	503	4/4	0.87	0.31	69,76,78,94	0
4	EDO	N	303	4/4	0.87	0.27	75,84,85,99	0
4	EDO	E	303	4/4	0.88	0.20	83,91,97,105	0
4	EDO	F	503	4/4	0.88	0.17	51,53,66,71	0
4	EDO	O	301	4/4	0.89	0.35	112,119,124,133	0
4	EDO	A	302	4/4	0.90	0.19	45,83,87,89	0
4	EDO	N	302	4/4	0.90	0.26	57,59,63,66	0
4	EDO	L	501	4/4	0.91	0.23	56,73,82,85	0
4	EDO	L	502	4/4	0.92	0.22	52,66,70,76	0
3	L3D	J	301	33/33	0.92	0.18	38,56,67,75	0
4	EDO	H	301	4/4	0.92	0.22	56,62,70,77	0
4	EDO	P	301	4/4	0.92	0.22	69,95,96,97	0
4	EDO	F	501	4/4	0.93	0.21	45,72,78,85	0
3	L3D	N	301	33/33	0.93	0.17	43,56,76,80	0
3	L3D	F	502	33/33	0.93	0.16	48,65,85,86	0
4	EDO	D	301	4/4	0.93	0.23	69,76,91,92	0
4	EDO	F	504	4/4	0.94	0.21	55,72,74,114	0
3	L3D	B	301	33/33	0.94	0.15	56,84,104,117	0
4	EDO	E	304	4/4	0.94	0.35	58,70,73,81	0
3	L3D	A	301	33/33	0.95	0.15	29,41,54,59	0
4	EDO	J	302	4/4	0.95	0.14	70,72,75,82	0
4	EDO	F	506	4/4	0.95	0.26	58,81,84,100	0
3	L3D	E	301	33/33	0.96	0.14	24,36,44,49	0
3	L3D	I	301	33/33	0.97	0.12	23,37,48,48	0
3	L3D	M	301	33/33	0.97	0.12	30,37,49,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

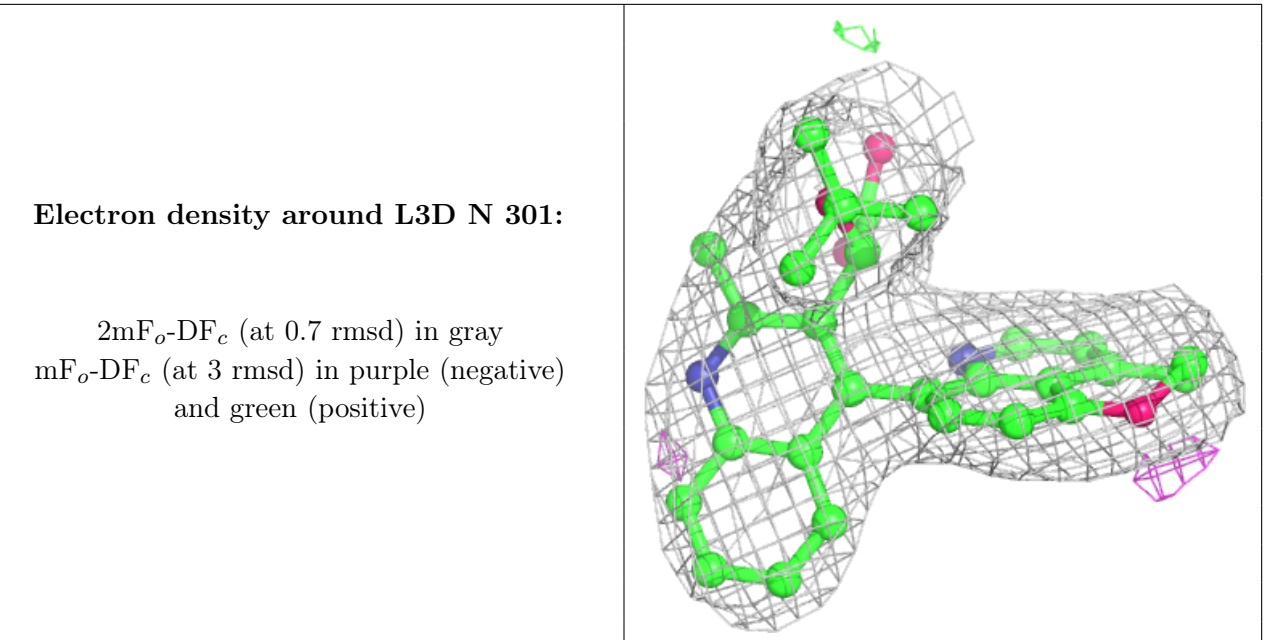
Electron density around L3D J 301:

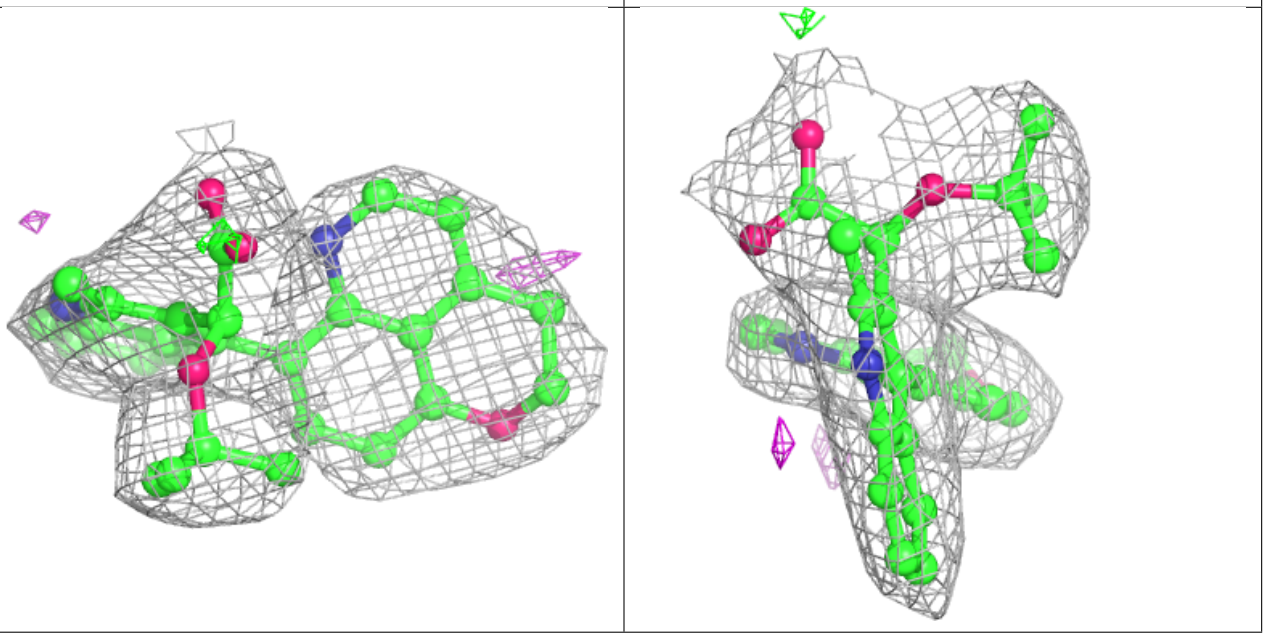
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around L3D N 301:

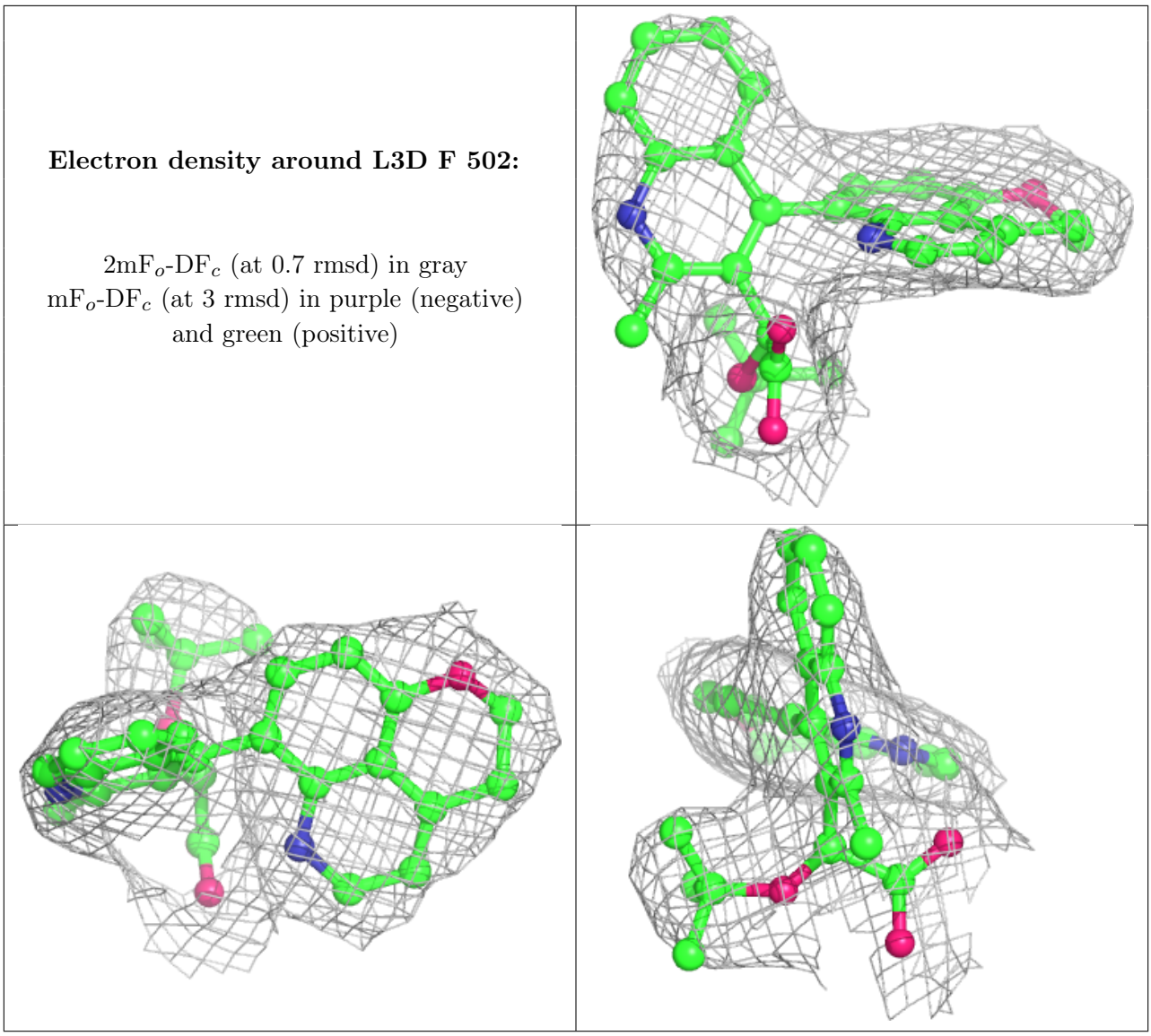
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





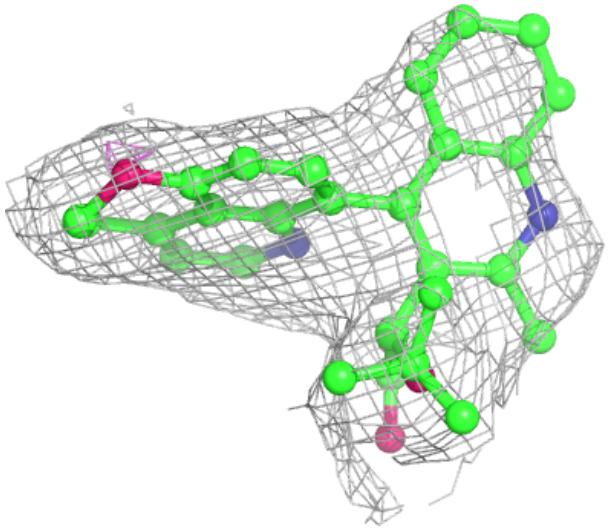
Electron density around L3D F 502:

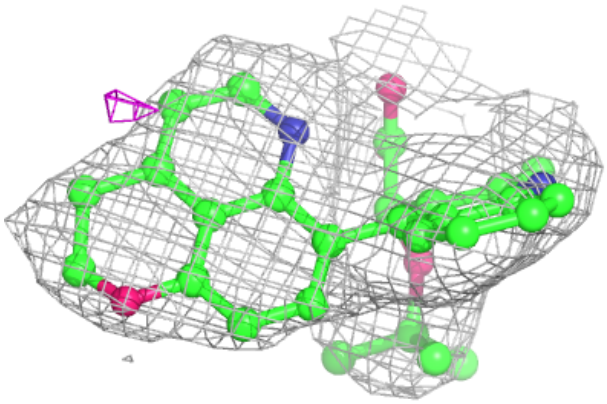
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

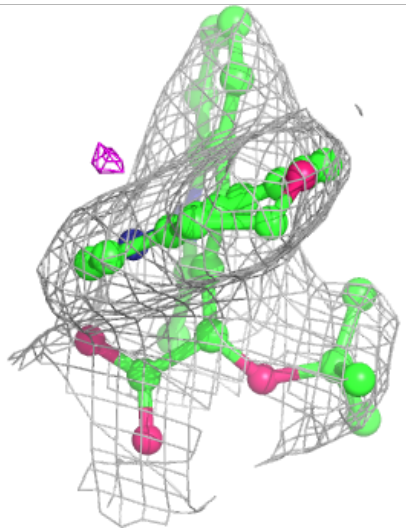


Electron density around L3D B 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

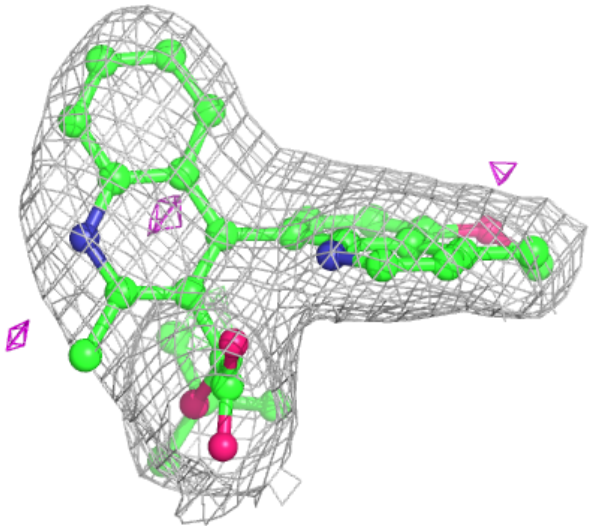


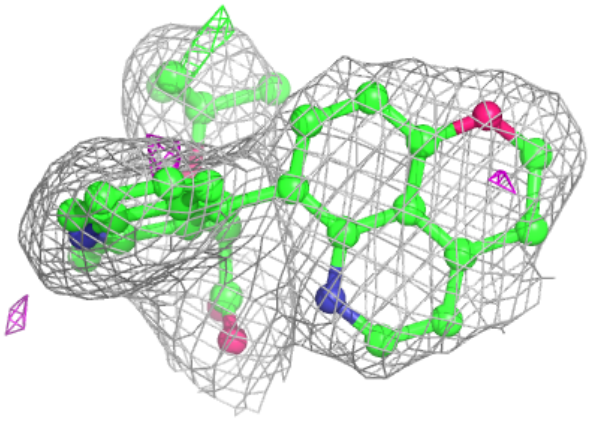


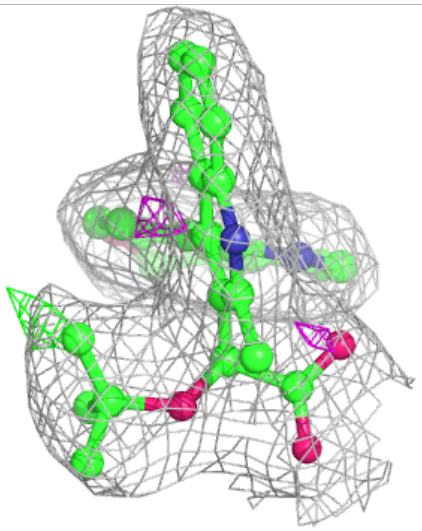


Electron density around L3D A 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

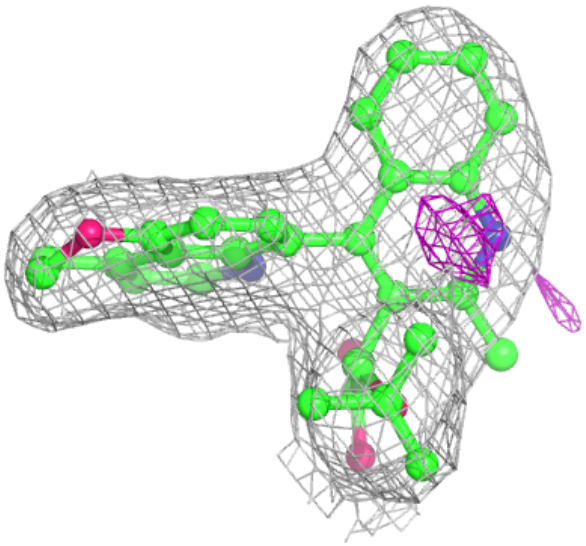


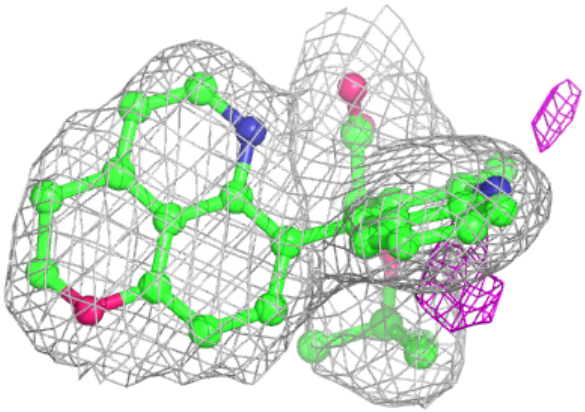


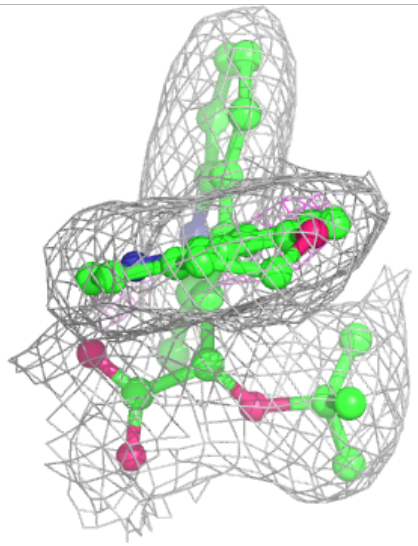


Electron density around L3D E 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

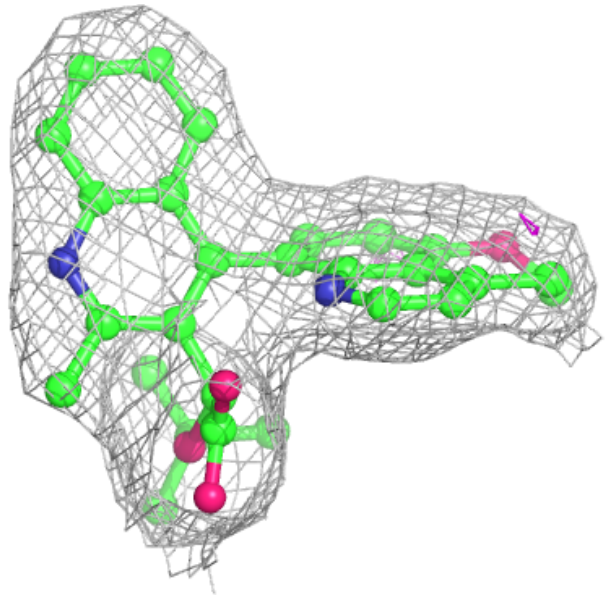


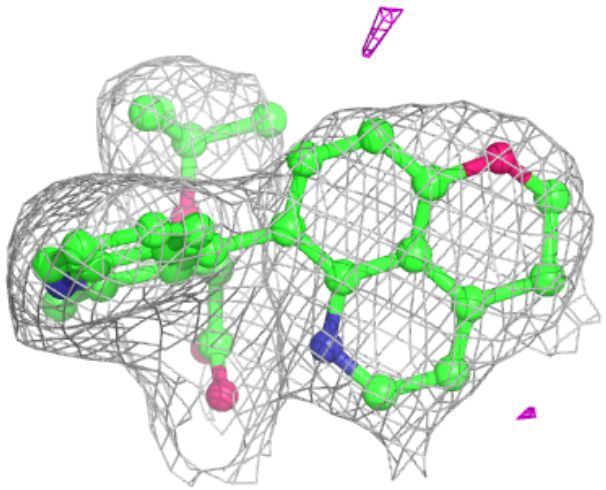


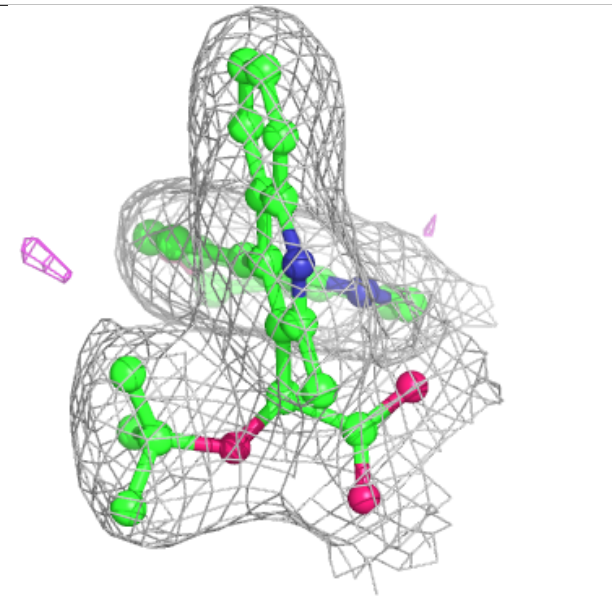


Electron density around L3D I 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

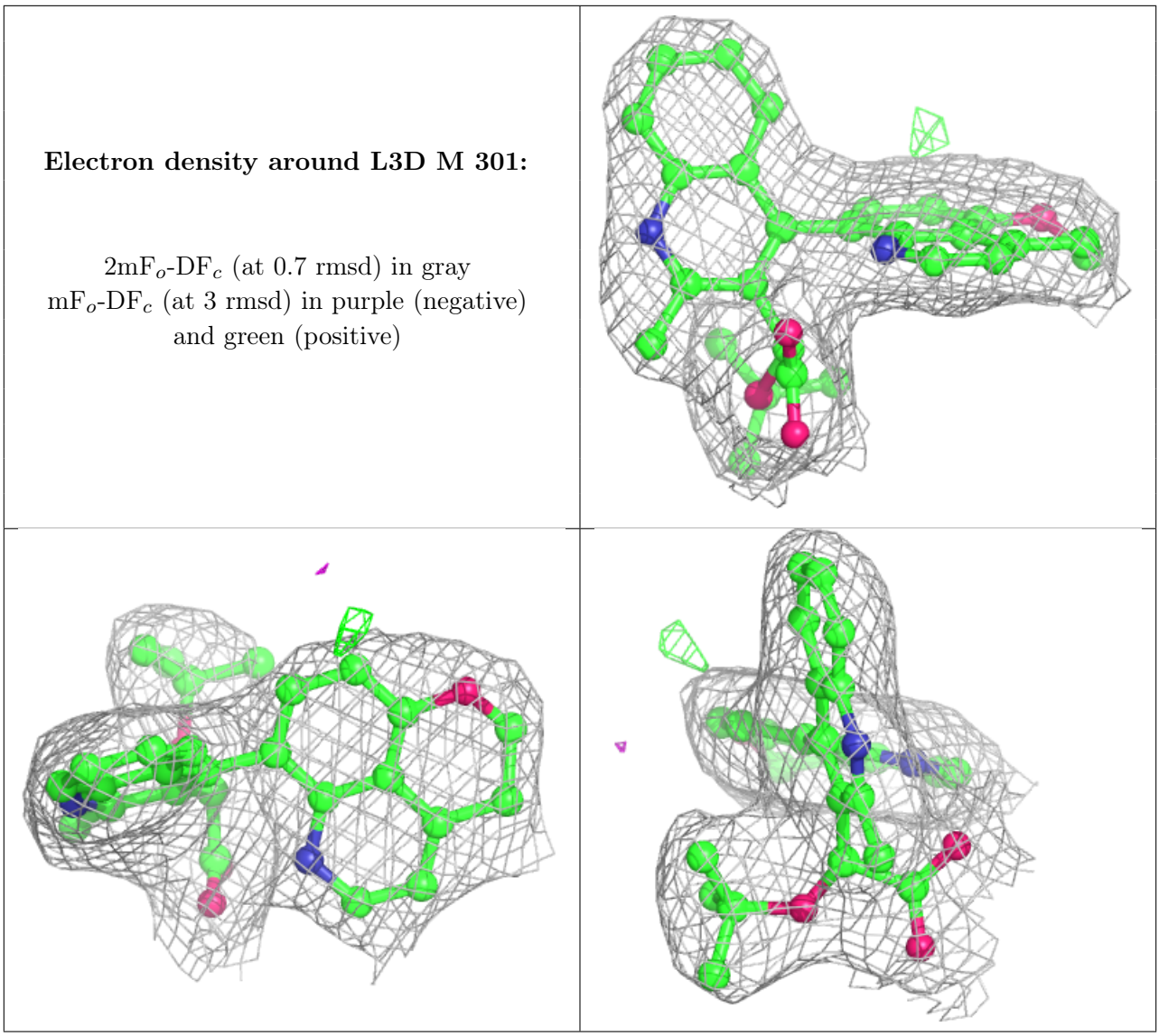






Electron density around L3D M 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.